

**MAX-PLANCK-INSTITUT FÜR WISSENSCHAFTSGESCHICHTE**

Max Planck Institute for the History of Science

2008

**PREPRINT 350**

Christian Joas, Christoph Lehner,  
and Jürgen Renn (eds.)

**HQ-1: Conference on the History  
of Quantum Physics**

**Max-Planck-Institut für Wissenschaftsgeschichte**  
Max Planck Institute for the History of Science

Christian Joas, Christoph Lehner, and Jürgen Renn (eds.)

# **HQ-1: Conference on the History of Quantum Physics**



**Preprint 350**

2008



This preprint volume is a collection of papers presented at HQ-1. The editors wish to thank Carmen Hammer, Nina Ruge, Judith Levy and Alexander Riemer for their substantial help in preparing the manuscript.

© MAX PLANCK INSTITUTE FOR THE HISTORY OF SCIENCE, 2008

NO REPRODUCTION ALLOWED. COPYRIGHT REMAINS WITH THE AUTHORS OF THE INDIVIDUAL ARTICLES. FRONT PAGE ILLUSTRATIONS: COPYRIGHT LAURENT TAUDIN.



## Preface

The present volume contains a selection of papers presented at the HQ-1 Conference on the History of Quantum Physics. This conference, held at the Max Planck Institute for the History of Science (July 2–6, 2007), has been sponsored by the Max Planck Society in honor of Max Planck on the occasion of the sixtieth anniversary of his passing. It is the first in a new series of conferences devoted to the history of quantum physics, to be organized by member institutions of the recently established International Project on the History and Foundations of Quantum Physics (Quantum History Project). The second meeting, HQ-2, takes place in Utrecht (July 14–17, 2008).

The Quantum History Project is an international cooperation of researchers interested in the history and foundations of quantum physics. It has been initiated jointly by the Fritz Haber Institute of the Max Planck Society (FHI) and the Max Planck Institute for the History of Science (MPIWG) and is being funded from the Strategic Innovation Fund of the President of the Max Planck Society. In addition to the FHI and the MPIWG, the primary institutions of the project are the Johns Hopkins University, the University of Notre Dame, the University of Minnesota, the University of Pittsburgh, the University of Rostock, and the Universidade Federal de Bahia, Brazil.

The aim of the Quantum History Project is to arrive at a deeper understanding of the genesis and development of quantum physics. While the main focus is on the birth of quantum mechanics in the period around 1925, the project also addresses further developments up to the present time, including the theoretical and experimental practices of quantum physics as well as debates about its foundations. The project is conceived as a close collaboration of a large and varied international group of historians and philosophers of science as well as working physicists.

Few scientific revolutions have drawn as much attention as the quantum revolution. We are fortunate that efforts in several places have built extensive archival records for historians to draw upon; and that some of the extant historical writings are models of scholarship. Parts of the existing literature, however, fail to meet the particular challenges of writing the history of quantum physics. Unlike the relativity revolution, the development of quantum physics was a communal effort whose nature cannot be easily captured by a biographical approach that focuses on a few central figures. Careful attention must be paid to the broader community of researchers and to how they could achieve together what no single researcher could do alone. Another problem is that not much of the existing literature is reliable when it comes to explaining crucial mathematical arguments in the primary source material. Finally, a sound understanding of the advent of quantum physics cannot be achieved without a subtle appreciation of the radical conceptual changes that it brought. Much of the conceptual analysis in historical writing on the quantum revolution uncritically presumes an unhistorical view of a unified Copenhagen interpretation. In fact, the history of the interpretation of quantum mechanics is, itself, a topic in need of more thorough and dispassionate historical investigation, all the more so because debates about interpretation played and continue to play an unusually prominent role in the development of quantum physics.

In view of these challenges, the Quantum History Project is conceived as a close collaboration of a large and varied international group of historians and philosophers of science and working physicists, reflected by the contributors to the present preprint vol-

## Preface

---

ume. Thus, the project takes advantage of the scientific expertise of the physicists and at the same time intends to reflect modern historiographical and philosophical approaches. It is based on the careful analysis of sources (published papers as well as correspondence, research manuscripts, and laboratory notebooks) and, where possible, instruments. Attention is also paid to the institutional and socio-cultural dimensions of the development of quantum physics.

The Quantum History Project aims at creating and fostering a collaborative climate and an infrastructure for scholarly research into the birth and development of quantum physics. We are actively establishing a network of scholars exchanging ideas and viewpoints through frequent and regular meetings (symposia, workshops, summer schools). In particular, we want to facilitate exchanges between physicists, historians, and philosophers interested in the history or the foundations of quantum physics. In addition, we make a special effort to draw young scholars into the project through graduate fellowships and postdoc positions. In support of these activities, we develop and maintain an easily accessible electronic resource base of both primary source material, published books and articles as well as archival material, and results of ongoing research by members of the network. We will likewise create an electronic educational resource for the dissemination of the history of quantum physics, creating and collecting materials accessible to a wide range of audiences, from the general public to graduate students in (history of) physics.

The aim of HQ-1 was to bring together scholars from different disciplines and countries who are experts in the conceptual and theoretical development of quantum physics, its experimental practice, and its institutional, philosophical and cultural context. Three areas were the main focus of the HQ-1 conference

- The old quantum theory: Its emergence of an array of seemingly unrelated problems in diverse areas such as statistical physics, radiation theory, and spectroscopy; how it was applied to an increasing number of problems; and how the physics community came to recognize its limitations.
- The genesis of modern quantum mechanics in the period around 1925, its conceptual development, the interplay with experiment, its socio-cultural and institutional context, as well as the debates about the different mathematical formulations of the theory (matrix and wave mechanics, transformation theory) and their physical interpretation (statistical interpretation, uncertainty principle).
- The acceptance of quantum mechanics as a new basis for physics (atomic, molecular, nuclear, and solid-state) and parts of chemistry; the elaboration of its mathematical formalism; the establishment of the dominant Copenhagen interpretation and the emergence of critical responses; and subsequent developments up to the present, including the ability to produce and control phenomena that until recently existed only as theoretical speculation.

Not all contributions to the HQ-1 conference are included in this two-volume preprint. The selection has not been based on a peer-review process but it rather was left open to each participant individually whether to submit a paper. The editors wish to stress the fact that the aim of the present preprint is not to assemble former or future publications of the participants but instead to provide a glimpse on recent developments in the

field via papers of preprint nature that reflect the status of research at the time of the conference. The copyright for the papers remains with the original authors who have to be contacted for permission of reproduction or any further use.

All papers have been carefully edited to conform a common L<sup>A</sup>T<sub>E</sub>X style. The editors apologize for any mistakes generated during this process and wish to thank Carmen Hammer, Nina Ruge, Judith Levy and Alexander Riemer for the considerable amount of time they invested into the completion of this two-volume preprint. We also wish to thank the other members of the Program Committee (Don Howard, Michel Janssen, John Norton, Robert Rynasiewicz) and all participants of HQ-1 for a fruitful conference.

The editors would like to dedicate this volume to the memory of Jürgen Ehlers (1929–2008). We felt very lucky and honored that a physicist of his importance took such an enthusiastic interest in our project. Jürgen Ehlers participated from the beginning of the project regularly in our meetings. He contributed not only with his scientific acumen, but also with his thoughtful sense of history and his wonderful personality to our group. We will miss him sorely.

Berlin, in June 2008,

Christian Joas  
Christoph Lehner  
Jürgen Renn



## Preface

---





## Preface

---



# Contents

## Volume 1

- 1 Einstein's Revolutionary Light-Quantum Hypothesis**  
ROGER H. STUEWER 1
- 2 The Odd Couple: Boltzmann, Planck and the Application of Statistics to Physics (1900–1913)**  
MASSIMILIANO BADINO 17
- 3 Poincaré's Electromagnetic Quantum Mechanics**  
ENRICO R. A. GIANNETTO 49
- 4 Einstein's Miraculous Argument of 1905: The Thermodynamic Grounding of Light Quanta**  
JOHN D. NORTON 63
- 5 The Ehrenfest Adiabatic Hypothesis and the Old Quantum Theory, before Bohr**  
ENRIC PÉREZ CANALS AND MARTA JORDI TALTAVULL 79
- 6 Re-Examining the Crisis in Quantum Theory, Part 1: Spectroscopy**  
DAVID C. CASSIDY 101
- 7 The Causality Debates of the Interwar Years and their Preconditions: Revisiting the Forman Thesis from a Broader Perspective**  
MICHAEL STÖLTZNER 113
- 8 Electron Spin or 'Classically Non-Describable Two-Valuedness'**  
DOMENICO GIULINI 127
- 9 First Steps (and Stumbles) of Bose-Einstein Condensation**  
DANIELA MONALDI 155

## Volume 2

- 10 Pascual Jordan's Resolution of the Conundrum of the Wave-Particle Duality of Light**  
ANTHONY DUNCAN AND MICHEL JANSSEN 165
- 11 Why Were Two Theories Deemed Logically Distinct, and Yet, Equivalent in**

## Contents

---

<b>Quantum Mechanics?</b> SLOBODAN PEROVIC	211
<b>12 Planck and de Broglie in the Thomson Family</b> JAUME NAVARRO	229
<b>13 Weyl Entering the 'New' Quantum Mechanics Discourse</b> ERHARD SCHOLZ	249
<b>14 The Statistical Interpretation According to Born and Heisenberg</b> GUIDO BACCIAGALUPPI	269
<b>15 Early Impact of Quantum Physics on Chemistry: George Hevesy's Work on Rare Earth Elements and Michael Polanyi's Absorption Theory</b> GABOR PALLO	289
<b>16 Computational Imperatives in Quantum Chemistry</b> BUHM SOON PARK	299
<b>17 A Service for the Physicists? B. L. van der Waerden's Early Contributions to Quantum Mechanics</b> MARTINA R. SCHNEIDER	323
<b>18 Engineering Entanglement: Quantum Computation, Quantum Communication, and Re-conceptualizing Information</b> CHEN-PANG YEANG	341

# 1 Einstein's Revolutionary Light-Quantum Hypothesis

ROGER H. STUEWER

*I sketch Albert Einstein's revolutionary conception of light quanta in 1905 and his introduction of the wave-particle duality into physics in 1909 and then offer reasons why physicists generally had rejected his light-quantum hypothesis by around 1913. These physicists included Robert A. Millikan, who confirmed Einstein's equation of the photoelectric effect in 1915 but rejected Einstein's interpretation of it. Only after Arthur H. Compton, as a result of six years of experimental and theoretical work, discovered the Compton effect in 1922, which Peter Debye also discovered independently and virtually simultaneously, did physicists generally accept light quanta. That acceptance, however, was delayed when George L. Clark and William Duane failed to confirm Compton's experimental results until the end of 1924, and by the publication of the Bohr-Kramers-Slater theory in 1924, which proposed that energy and momentum were conserved only statistically in the interaction between a light quantum and an electron, a theory that was not disproved experimentally until 1925, first by Walter Bothe and Hans Geiger and then by Compton and Alfred W. Simon.*

## Light Quanta

Albert Einstein signed his paper, "Concerning a Heuristic Point of View about the Creation and Transformation of Light,"<sup>1</sup> in Bern, Switzerland, on March 17, 1905, three days after his twenty-sixth birthday. It was the only one of Einstein's great papers of 1905 that he himself called "very revolutionary."<sup>2</sup> As we shall see, Einstein was correct: His light-quantum hypothesis was not generally accepted by physicists for another two decades.

Einstein gave two arguments for light quanta, a negative and a positive one. His negative argument was the failure of the classical equipartition theorem, what Paul Ehrenfest later called the "ultraviolet catastrophe."<sup>3</sup> His positive argument proceeded in two stages. First, Einstein calculated the change in entropy when a volume  $V_0$  filled with blackbody radiation of total energy  $U$  in the Wien's law (high-frequency) region of the spectrum was reduced to a subvolume  $V$ . Second, Einstein used Boltzmann's statistical version of the entropy to calculate the probability of finding  $n$  independent, distinguishable gas molecules moving in a volume  $V_0$  at a given instant of time in a

---

<sup>1</sup>Einstein (1905).

<sup>2</sup>Einstein to Conrad Habicht, May 18 or 25, 1905. In Klein, Kox, and Schulmann (1993), p. 31; Beck (1995), p. 20.

<sup>3</sup>Quoted in Klein (1970), pp. 249–250.

subvolume  $V$ . He found that these two results were formally identical, providing that

$$U = n \left( \frac{R\beta}{n} \right) \nu,$$

where  $R$  is the ideal gas constant,  $\beta$  is the constant in the exponent in Wien's law,  $N$  is Avogadro's number, and  $\nu$  is the frequency of the radiation. Einstein concluded:

“Monochromatic radiation of low density (within the range of validity of Wien's radiation formula) behaves thermodynamically as if it consisted of mutually independent energy quanta of magnitude  $R\beta\nu/N$ .”<sup>4</sup>

Einstein cited three experimental supports for his light-quantum hypothesis, the most famous one being the photoelectric effect, which was discovered by Heinrich Hertz at the end of 1886<sup>5</sup> and explored in detail experimentally by Philipp Lenard in 1902.<sup>6</sup> Einstein wrote down his famous equation of the photoelectric effect,

$$\Pi e = \left( \frac{R}{N} \right) \beta \nu - P,$$

where  $\Pi$  is the potential required to stop electrons (charge  $e$ ) from being emitted from a photosensitive surface after their energy had been reduced by its work function  $P$ . It would take a decade to confirm this equation experimentally. Einstein also noted, however, that if the incident light quantum did not transfer all of its energy to the electron, then the above equation would become an inequality:

$$\Pi e < \left( \frac{R}{N} \right) \beta \nu - P.$$

It would take almost two decades to confirm this equation experimentally.

We see, in sum, that Einstein's arguments for light quanta were based upon Boltzmann's statistical interpretation of the entropy. He did not propose his light-quantum hypothesis “to explain the photoelectric effect,” as physicists today are fond of saying. As noted above, the photoelectric effect was only one of three experimental supports that Einstein cited for his light-quantum hypothesis, so to call his paper his “photoelectric-effect paper” is completely false historically and utterly trivializes his achievement.

In January 1909 Einstein went further by analyzing the energy and momentum fluctuations in black-body radiation.<sup>7</sup> He now assumed the validity of Planck's law and showed that the expressions for the mean-square energy and momentum fluctuations split naturally into a sum of two terms, a wave term that dominated in the Rayleigh-Jeans (low-frequency) region of the spectrum and a particle term that dominated in the Wien's law (high-frequency) region. This constituted Einstein's introduction of the wave-particle duality into physics.<sup>8</sup>

Einstein presented these ideas again that September in a talk he gave at a meeting of the Gesellschaft Deutscher Naturforscher und Ärzte in Salzburg, Austria.<sup>9</sup> During

---

<sup>4</sup>Einstein (1905), p. 143. In Stachel (1989), p. 161; Beck (1989), p. 97.

<sup>5</sup>For discussions, see Stuewer (1971); Buchwald (1994), pp. 243–244.

<sup>6</sup>Lenard (1902).

<sup>7</sup>Einstein (1909a).

<sup>8</sup>Klein (1964). For the wave-particle duality placed in a new context, see Duncan and Janssen (2007).

<sup>9</sup>Einstein (1909b).

the discussion, Max Planck took the acceptance of Einstein's light quanta to imply the rejection of Maxwell's electromagnetic waves which, he said, "seems to me to be a step which in my opinion is not yet necessary."<sup>10</sup> Johannes Stark was the only physicist at the meeting who supported Einstein's light-quantum hypothesis.<sup>11</sup>

In general, by around 1913 most physicists rejected Einstein's light-quantum hypothesis, and they had good reasons for doing so. First, they believed that Maxwell's electromagnetic theory had to be universally valid to account for interference and diffraction phenomena. Second, Einstein's statistical arguments for light quanta were unfamiliar to most physicists and were difficult to grasp. Third, between 1910 and 1913 three prominent physicists, J.J. Thomson, Arnold Sommerfeld, and O.W. Richardson, showed that Einstein's equation of the photoelectric effect could be derived on classical, non-Einsteinian grounds, thereby obviating the need to accept Einstein's light-quantum hypothesis as an interpretation of it.<sup>12</sup> Fourth, in 1912 Max Laue, Walter Friedrich, and Paul Knipping showed that X rays can be diffracted by a crystal,<sup>13</sup> which all physicists took to be clear proof that they were electromagnetic waves of short wavelength. Finally, in 1913 Niels Bohr insisted that when an electron underwent a transition in a hydrogen atom, an electromagnetic wave, not a light quantum, was emitted—a point to which I shall return later.

### Millikan's Photoelectric-Effect Experiments

Robert Andrews Millikan began working intermittently on the photoelectric effect in 1905 but not in earnest until October 1912, which, he said, then "occupied practically all of my individual research time for the next three years."<sup>14</sup> Earlier that spring he had attended Planck's lectures in Berlin, who he recalled, "very definitely rejected the notion that light travels through space in the form of bunches of localized energy." Millikan therefore "scarcely expected" that his experiments would yield a "positive" result, but "the question was very vital and an answer of some sort had to be found."

Millikan recalled that by "great good fortune" he eventually found "the key to the whole problem," namely, that radiation over a wide range of frequencies ejected photoelectrons from the highly electropositive alkali metals, lithium, sodium, and potassium. He then modified and improved his experimental apparatus until it became "a machine shop in vacuo." He reported his results at a meeting of the American Physical Society in Washington, D.C., in April 1915; they were published in *The Physical Review* in March 1916.<sup>15</sup> His data points fell on a perfectly straight line of slope  $h/e$  (Fig. 1.1), leaving no doubt whatsoever about the validity of Einstein's equation of the photoelectric effect.

That left the theoretical interpretation of his experimental results. In his Autobiography, which he published in 1950 at the age of 82, Millikan included a chapter entitled "The Experimental Proof of the Existence of the Photon," in which he wrote:

"This seemed to me, as it did to many others, a matter of very great im-

---

<sup>10</sup>Planck, "Discussion." In Einstein (1909b), p. 825; Stachel (1989), p. 585; Beck (1989), p. 395.

<sup>11</sup>Stark, "Discussion." In Einstein (1909b), p. 826; Stachel (1989), p. 586; Beck (1989), p. 397.

<sup>12</sup>Stuewer (1975), pp. 48–68.

<sup>13</sup>Friedrich, Knipping, and Laue (1912); Laue (1912). In Laue (1961), pp. 183–207, 208–218.

<sup>14</sup>Millikan (1950), p. 100.

<sup>15</sup>Millikan (1916).



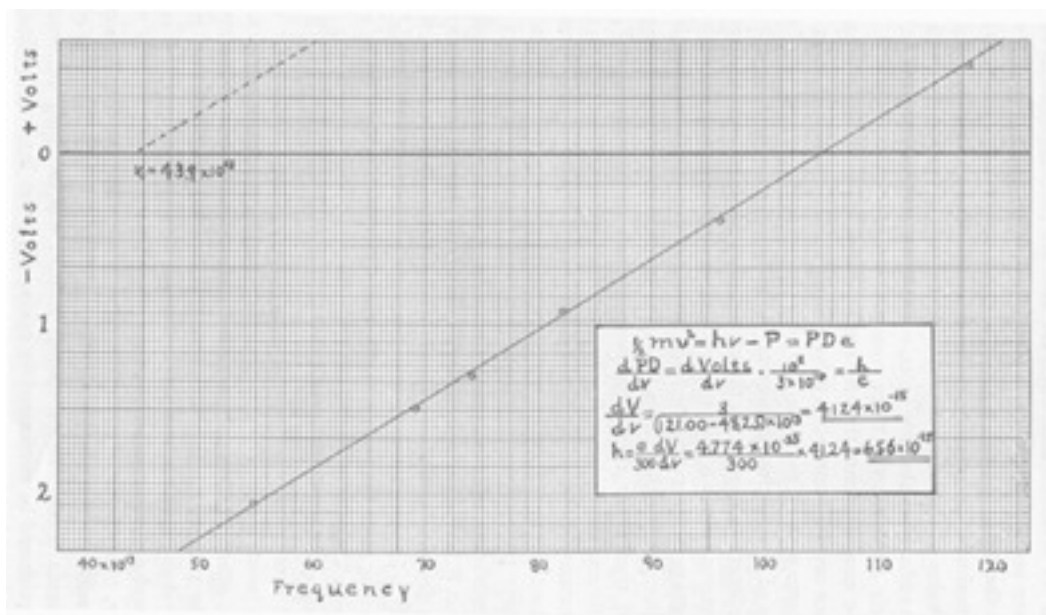


Figure 1.1: Millikan’s plot of the potential  $V$  required to stop photoelectrons from being ejected from sodium by radiation of frequency  $h/e$ . The plot is a straight line of slope  $h/e$ , in agreement with Einstein’s equation. *Source:* Millikan (1916), p. 373.

portance, for it . . . proved simply and irrefutably I thought, *that the emitted electron that escapes with the energy  $h\nu$  gets that energy by the direct transfer of  $h\nu$  units of energy from the light to the electron* and hence scarcely permits of any other interpretation than that which Einstein had originally suggested, namely that of the semi-corpuseular or photon theory of light itself [Millikan’s italics].”<sup>16</sup>

In Millikan’s paper of 1916, however, which he published at the age of 48, we find a very different interpretation. There Millikan declares that Einstein’s “bold, not to say reckless” light-quantum hypothesis “flies in the face of the thoroughly established facts of interference,”<sup>17</sup> so that we must search for “a substitute for Einstein’s theory.”<sup>18</sup> Millikan’s “substitute” theory was that the photosensitive surface must contain “oscillators of all frequencies” that “are at all times . . . loading up to the value  $h\nu$ .” A few of them will be “in tune” with the frequency of the incident light and thus will absorb energy until they reach that “critical value,” at which time an “explosion” will occur and electrons will be “shot out” from the atom.

Millikan therefore fell completely in line with J.J. Thomson, Sommerfeld, and Richardson in proposing a classical, non-Einsteinian theory of the photoelectric effect in his paper of 1916. No one, in fact, made Millikan’s views on Einstein’s light-quantum hypothesis clearer than Millikan himself did in his book, *The Electron*, which he published in 1917, where he wrote:

<sup>16</sup>Millikan (1950), pp. 101–102.

<sup>17</sup>Millikan (1916), p. 355.

<sup>18</sup>Ibid., p. 385.

Despite ... the apparently complete success of the Einstein equation, the physical theory of which it was designed to be the symbolic expression is found so untenable that Einstein himself, I believe, no longer holds to it, and we are in the position of having built a very perfect structure and then knocked out entirely the underpinning without causing the building to fall. It [Einstein's equation] stands complete and apparently well tested, but without any visible means of support. These supports must obviously exist, and the most fascinating problem of modern physics is to find them. Experiment has outrun theory, or, better, *guided by erroneous theory*, it has discovered relationships which seem to be of the greatest interest and importance, but the reasons for them are as yet not at all understood [my italics].<sup>19</sup>

This, note, is the same man who thirty-four years later, in 1950, wrote that his experiments “proved simply and irrefutably I thought,” that they scarcely permitted “any other interpretation than that which Einstein had originally suggested, namely that of the semi-corpuscular or photon theory of light.”

Historians have a name for this, namely, “revisionist history.” But this was by no means the first time that Millikan revised history as it suited him. The earliest instance I have found was his reproduction of a picture of J.J. Thomson in his study at home in Cambridge, England, sitting in a chair once owned by James Clerk Maxwell. Let us compare the original picture of 1899 with Millikan's reproduction of it in 1906 (Fig. 1.2). Note how Millikan has carefully etched out the cigarette in J.J.'s left hand. He presumably did not want to corrupt young physics students at the University of Chicago and elsewhere. In any case, this reflects what I like to call Millikan's philosophy of history: “If the facts don't fit your theory, change the facts.”

### Compton's Scattering Experiments<sup>20</sup>

Millikan's rejection of Einstein's light-quantum hypothesis characterized the general attitude of physicists toward it around 1916, when Arthur Holly Compton entered the field. Born in Wooster, Ohio, in 1892, Compton received his B.A. degree from the College of Wooster in 1913 and his Ph.D. degree from Princeton University in 1916. He then was an Instructor in Physics at the University of Minnesota in Minneapolis for one year (1916–1917), a Research Engineer at the Westinghouse Electric and Manufacturing Company in Pittsburgh for two years (1917–1919), and a National Research Council Fellow at the Cavendish Laboratory in Cambridge, England, for one year (1919–1920) before accepting an appointment as Wayman Crow Professor and Head of the Department of Physics at Washington University in St. Louis in the summer of 1920, where he remained until moving to the University of Chicago three years later.

While at Westinghouse in Pittsburgh, Compton came across a puzzling observation that Charles Grover Barka made in 1917,<sup>21</sup> namely, that the mass-absorption coefficient of 0.145-Angstrom X rays in aluminum was markedly smaller than the Thomson mass-scattering coefficient whereas it should have been larger. To explain this, Compton

---

<sup>19</sup>Millikan (1917), p. 230.

<sup>20</sup>For a full discussion, see Stuewer (1975).

<sup>21</sup>Barkla and White (1917); Stuewer (1975), pp. 96–103.

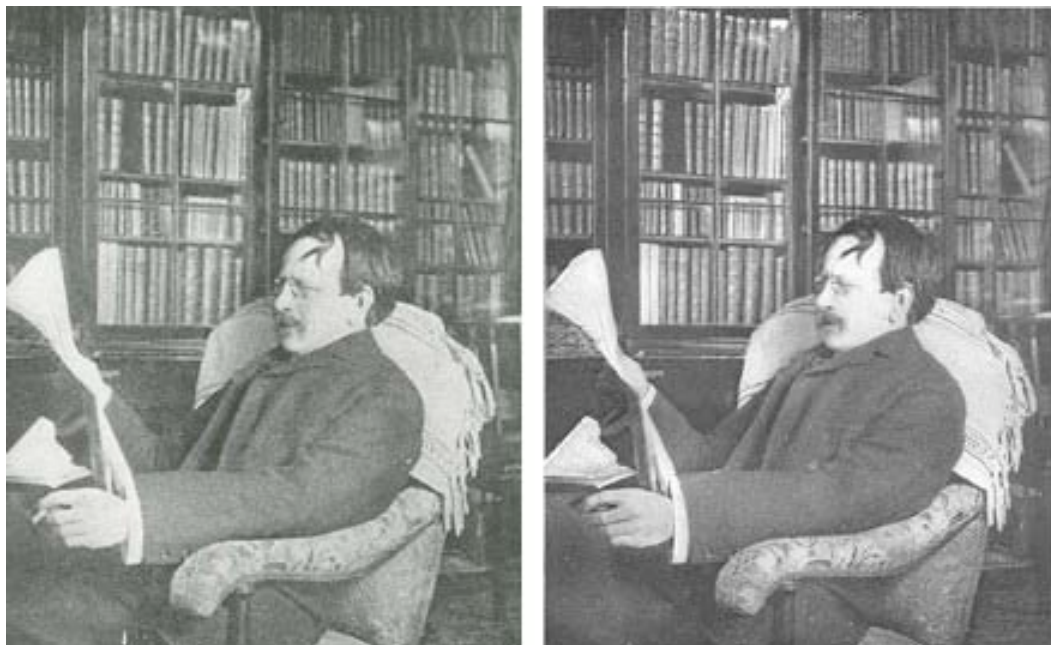


Figure 1.2: Left panel: J.J. Thomson (1856–1940) seated in a chair once owned by James Clerk Maxwell (1831–1879) as seen in a photograph of 1899. *Source:* Thomson, George Paget (1964), facing p. 53. Right panel: The same photograph as reproduced by Robert A. Millikan (1868–1953) in 1906. Note how carefully Millikan has etched out the cigarette in J.J.’s left hand. *Source:* Millikan and Gale (1906), facing p. 482.

eventually concluded that the X rays were being *diffracted* by electrons in the aluminum atoms, which demanded that the diameter of the electron be on the order of the wavelength of the incident X rays, say  $0.1 \text{ \AA}$ —in other words, nearly as large as the Bohr radius of the hydrogen atom, which was an exceedingly large electron. That was too much for Ernest Rutherford, who after Compton moved to the Cavendish Laboratory and gave a talk at a meeting of the Cambridge Philosophical Society, introduced Compton with the words: “This is Dr. Compton who is here to talk to us about the Size of the Electron. Please listen to him attentively, but you don’t have to believe him.”<sup>22</sup> Charles D. Ellis recalled that at one point in Compton’s talk Rutherford burst out saying, “I will not have an electron in my laboratory as big as a balloon!”<sup>23</sup>

Compton, in fact, eventually abandoned his large-electron scattering theory to a considerable degree as a consequence of gamma-ray experiments that he carried out at the Cavendish Laboratory.<sup>24</sup> He found that (1) the intensity of the scattered  $\gamma$  rays was greater in the forward than in the reverse direction; (2) the scattered  $\gamma$  rays were “softer” or of greater wavelength than the primary  $\gamma$ -rays; (3) the “hardness” or wavelength of the scattered  $\gamma$  rays was independent of the nature of the scatterer; and (4) the scattered  $\gamma$  rays became “softer” or of greater wavelength as the scattering angle increased.

We recognize these as exactly the characteristics of the Compton effect, but the ques-

---

<sup>22</sup>Quoted in Compton (1967), p. 29.

<sup>23</sup>Quoted in Eve (1939), p. 285.

<sup>24</sup>Stuewer (1975), pp. 135–158.

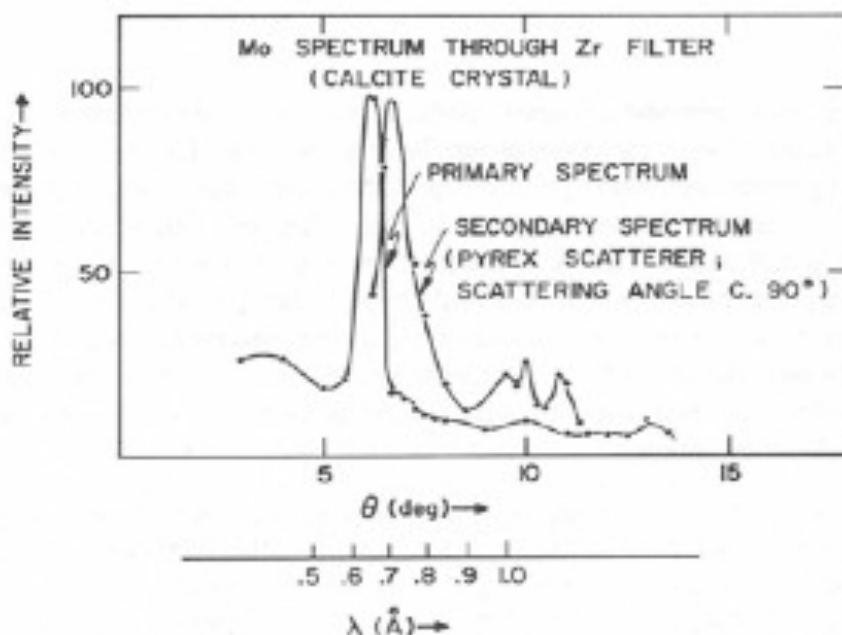


Figure 1.3: Author's plot of Compton's spectra of December 1921 for Molybdenum  $K_{\alpha}$  X rays scattered by Pyrex through an angle of about  $90^{\circ}$ . *Source*: Stuewer (1975), p. 187.

tion is: How did Compton explain these striking experimental results in 1919? The answer is that Compton, like virtually every other physicist at this time, also was completely convinced that  $\gamma$  rays and X rays were electromagnetic radiations of short wavelength. And after much thought, he hit on the idea that the electrons in the scatterer were tiny oscillators that the incident  $\gamma$  rays were propelling forward at high velocities, causing the electrons to emit a new type of secondary "fluorescent" radiation. The intensity of this secondary radiation would be peaked in the forward direction, and its increased wavelength was due to the Doppler effect.

Compton left the Cavendish Laboratory in the summer of 1920, taking a Bragg spectrometer along with him, because he knew that he wanted to carry out similar X-ray experiments at Washington University in St. Louis.<sup>25</sup> He obtained his first X-ray spectra in December 1921 by sending Molybdenum  $K_{\alpha}$  X rays (wavelength  $\lambda = 0.708 \text{ \AA}$ ) onto a Pyrex scatterer and observing the scattered X rays at a scattering angle of about  $90^{\circ}$  (Fig. 1.3). I emphasize that these are my plots of Compton's data as recorded in his laboratory notebooks, because I knew what I was looking for, namely, the small change in wavelength between the primary and secondary peaks, while Compton did not know what he was looking for, and—as his published paper makes absolutely clear—saw these two high peaks as the single primary peak, and the low peak at a wavelength of  $\lambda' = 0.95 \text{ \AA}$  as the secondary peak, whose wavelength thus was about 35% greater than that of the primary peak. Compton therefore concluded that the ratio of the wavelength  $\lambda$  of the primary peak to the wavelength  $\lambda'$  of the secondary peak was  $\lambda/\lambda' = (0.708 \text{ \AA})/(0.95 \text{ \AA}) = 0.75$ .

<sup>25</sup>Stuewer (1975), pp. 158–215.

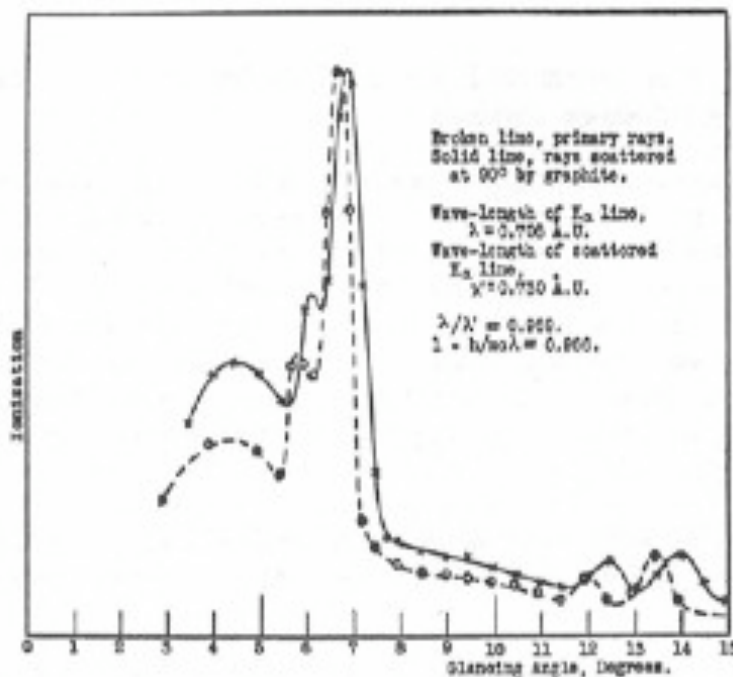


Figure 1.4: Compton's spectra of October 1922 for Molybdenum  $K_\alpha$  X rays scattered by graphite (carbon) through an angle of  $90^\circ$ . *Source:* Compton (1922), p. 16; Shankland (1973), p. 336.

The question is: How did Compton interpret this experimental result theoretically? Answer: By invoking the Doppler effect, which at  $90^\circ$  is expressed as  $\lambda/\lambda' = 1 - v/c$ , where  $v$  is the velocity of the electron and  $c$  is the velocity of light. To eliminate the velocity  $v$  of the electron, Compton then invoked what he regarded as “conservation of energy,” namely, that  $\frac{1}{2}mv^2 = h\nu$ , where  $m$  is the rest mass of the electron, so that  $\lambda/\lambda' = 1 - v/c = 1 - [(2h\nu)/(mv^2)]^{1/2}$ , or substituting numbers,  $\lambda/\lambda' = 1 - [(2(0.17 \text{ MeV})/(0.51 \text{ MeV}))^{1/2}] = 1 - 0.26 = 0.74$ . Who could ask for better agreement between theory and experiment? I think this is a wonderful historical example of a false theory being confirmed by spurious experimental data.

By October 1922, however, Compton knew that the change in wavelength was not 35% but only a few percent.<sup>26</sup> By then he had sent Molybdenum  $K_\alpha$  X rays onto a graphite (carbon) scatterer and observed the scattered X rays at a scattering angle of  $90^\circ$  (Fig. 1.4), finding that the wavelength  $\lambda'$  of the secondary peak was  $\lambda' = 0.730 \text{ \AA}$ , so that now  $\lambda/\lambda' = (0.708 \text{ \AA})/(0.730 \text{ \AA}) = 0.969$ .

The question again is: How did Compton interpret this experimental result theoretically? Answer: By again invoking the Doppler effect, namely, that at  $90^\circ$   $\lambda/\lambda' = 1 - v/c$ , where now to eliminate the velocity  $v$  of the electron, Compton invoked what he regarded as “conservation of momentum,” namely, that  $mv = h/\lambda$ , so that  $\lambda/\lambda' = 1 - v/c = 1 - h/mc^2$ , which is exactly the equation he placed to the right of his spectra. Rewriting it as  $\lambda/\lambda' = 1 - h\nu/mv^2$  and substituting numbers, he found that

<sup>26</sup>Compton (1922).

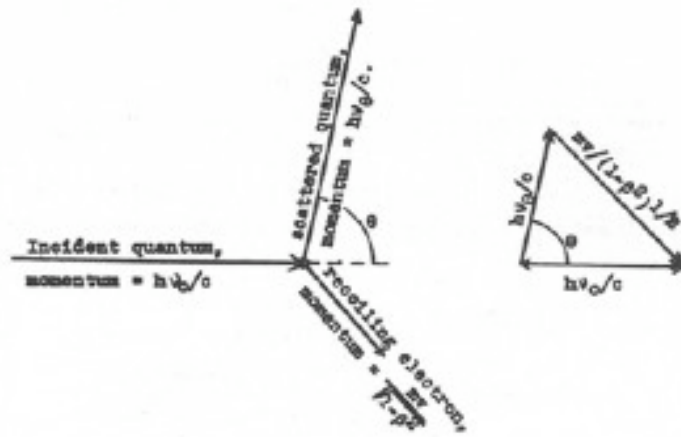


Figure 1.5: Compton's quantum theory of scattering of 1922. A primary X-ray quantum of momentum  $h\nu_0/c$  strikes an electron and scatters through an angle  $\theta$ , producing a secondary X-ray quantum of momentum  $h\nu_\theta/c$  and propelling the electron away with a relativistic momentum of  $mv/\sqrt{1-\beta^2}$ , where  $m$  is the rest mass of the electron and  $\beta = v/c$ . *Source:* Compton (1923), 486; Shankland (1975), p. 385.

$\lambda/\lambda' = 1 - (0.17 \text{ MeV})/(0.51 \text{ MeV}) = 1 - 0.034 = 0.966$ . Again, who could ask for better agreement between theory and experiment? I think this is a wonderful historical example of a false theory being confirmed by good experimental data.

Compton put everything together one month later, in November 1922, aided materially by discussions he had had with his departmental colleague G.E.M. Jauncey.<sup>27</sup> He now assumed that an X-ray quantum strikes an electron in a billiard-ball collision process in which both energy and momentum are conserved.<sup>28</sup> He drew his famous vector diagram (Fig. 1.5) and calculated the change in wavelength

$$\Delta\lambda = \lambda_\theta - \lambda_0 = \frac{h}{mc}(1 - \cos\theta) = \frac{h}{mc}$$

between the incident and scattered light quantum for a scattering angle of  $\theta = 90^\circ$ . What experimental support did Compton now cite for his new quantum theory of scattering? Note that the spectra he published in his paper of May 1923 (Fig. 1.6) were *identical* to those he had published in October 1922. Only his theoretical calculation to their right had changed. As every physicist knows, theories come and go, but good experimental data never dies!

We see that Compton's discovery of the Compton effect was the culmination of six years of experimental and theoretical research, between 1916 and 1922. His thought, in other words, evolved along with his own experimental and theoretical work, in a largely autonomous fashion. There is no indication, in particular, that Compton ever read Einstein's light-quantum paper of 1905. In fact, Compton neither cited Einstein's paper in his own paper of 1923, nor even mentioned Einstein's name in it.

This is in striking contrast to Peter Debye, who proposed the identical billiard-ball

<sup>27</sup>Jenkin (2002), pp. 328–330.

<sup>28</sup>Compton (1923a).

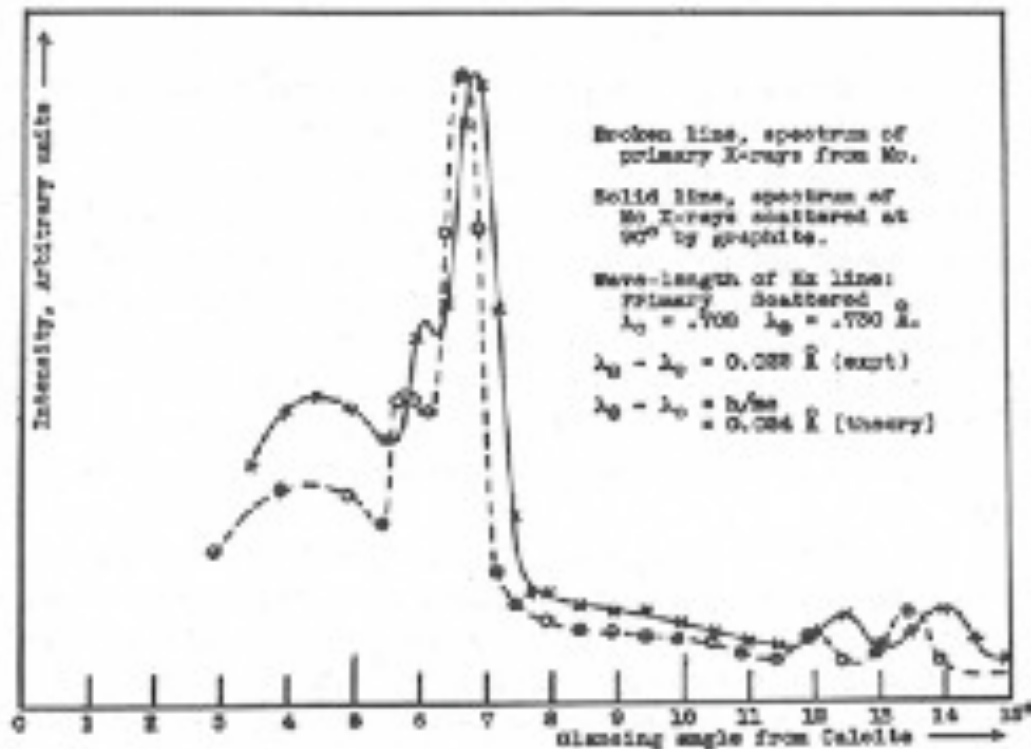


Figure 1.6: Compton's spectra of 1923 for Molybdenum  $K_\alpha$  X rays scattered by graphite (carbon) through an angle of  $90^\circ$ . Note that they are identical to those he published in October 1922 (Fig. 1.4), but that he now calculated the change in wavelength  $\lambda_\theta - \lambda_0 = h/mc$  between the secondary and primary light quantum on the basis of his new quantum theory of scattering. Source: Compton (1923), p. 495; Shankland (1975), p. 394.

quantum theory of scattering independently and virtually simultaneously,<sup>29</sup> and who explicitly stated in his paper that his point of departure was Einstein's concept of "needle radiation." The chronology of Compton's and Debye's work is instructive, as follows:

- *November 1922*: Compton reported his discovery to his class at Washington University.
- *December 1 or 2, 1922*: Compton reported his discovery at a meeting of the American Physical Society in Chicago.
- *December 6, 1922*: Compton submitted another paper, on the total-internal reflection of X rays, to the *Philosophical Magazine*.<sup>30</sup>
- *December 10, 1922*: Compton submitted his paper on his quantum theory of scattering to *The Physical Review*.

<sup>29</sup>Debye (1923).

<sup>30</sup>Compton (1923b).

- *March 15, 1923*: Debye submitted his paper on the quantum theory of scattering to the *Physikalische Zeitschrift*.
- *April 15, 1923*: Debye's paper was published in the *Physikalische Zeitschrift*.
- *May 1923*: Compton's paper was published in *The Physical Review*.

Now, there is nothing more wave-like than total-internal reflection, and there is nothing more particle-like than the Compton effect. We thus see that within the space of one week, between December 6 and December 10, 1922, Compton submitted for publication conclusive experimental evidence for *both* the wave *and* the particle nature of X rays. I take this to be symbolic of the profound dilemma that physicists faced at this time over the nature of radiation.

Further, as seen in the above chronology, Debye's paper actually appeared in print one month before Compton's, which led some physicists, especially European physicists, to refer to the discovery as the Debye effect or the Debye-Compton effect. Fortunately for Compton, Arnold Sommerfeld was in the United States at this time as a visiting professor at the University of Wisconsin in Madison, and because he knew that Compton had priority in both the experiment and the theory, after he returned home to Munich, Germany, he was instrumental in persuading European physicists that it should be called the Compton effect. Debye himself later insisted that it should be called the Compton effect, saying that the physicist who did most of the work should get the name.<sup>31</sup>

## Aftermath

Compton's experimental results, however, did not go unchallenged.<sup>32</sup> In October 1923 George L. Clark, a National Research Council Fellow working in William Duane's laboratory at Harvard University, announced—with Duane's full support—that he could not obtain the change in wavelength that Compton had reported. This was a serious experimental challenge to Compton's work, which was not resolved until December 1924 when Duane forthrightly admitted at a meeting of the American Physical Society that their experiments were faulty.<sup>33</sup>

That resolved the experimental question, but the theoretical question still remained open. Niels Bohr challenged Compton's quantum theory of scattering directly in early 1924. Bohr, in fact, had never accepted Einstein's light quanta. Most recently, in his Nobel Lecture in December 1922, Bohr had declared:

In spite of its heuristic value, . . . the hypothesis of light-quanta, which is quite irreconcilable with so-called interference phenomena, is not able to throw light on the nature of radiation.<sup>34</sup>

Two years later, in 1924, Bohr and his assistant Hendrik A. Kramers adopted John C. Slater's concept of virtual radiation and published, entirely without Slater's cooperation,

---

<sup>31</sup>Quoted in Kuhn and Uhlenbeck (1962), p. 12.

<sup>32</sup>Stuewer (1975), pp. 249–273.

<sup>33</sup>Bridgman (1936), p. 32.

<sup>34</sup>Bohr (1923 [1922]), p. 4; 14; 470.



the Bohr-Kramers-Slater paper<sup>35</sup> whose essential feature was that energy and momentum were conserved only statistically in the interaction between an incident light quantum and an electron in the Compton effect. As C.D. Ellis remarked, “it must be held greatly to the credit of this theory that it was sufficiently precise in its statements to be disproved definitely by experiment.”<sup>36</sup>

Hans Geiger and Walter Bothe in Berlin were the first to disprove the BKS theory, in coincidence experiments that they reported on April 18 and 25, 1925.<sup>37</sup> Then Compton (now at Chicago) and his student Alfred W. Simon disproved the BKS theory in even more conclusive coincident experiments that they reported on June 23, 1925. Even before that, however, on April 21, 1925, just after Bohr learned about the Bothe-Geiger results, he added a postscript to a letter to Ralph H. Fowler in Cambridge: “It seems therefore that there is nothing else to do than to give our revolutionary efforts as honourable a funeral as possible.”<sup>38</sup> Of course, as Einstein said in a letter of August 18, 1925, to his friend Paul Ehrenfest: “We both had no doubts about it.”<sup>39</sup>

## References

- Barkla, C.G. and White, M.P. (1917). “Notes on the Absorption and Scattering of X-rays and the Characteristic Radiation of *J*-series.” *Philosophical Magazine* **34**, 270–285.
- Beck, Anna, transl. (1989). *The Collected Papers of Albert Einstein*. Vol. 2. *The Swiss Years: Writings, 1900–1909*. Princeton: Princeton University Press.
- Beck, Anna, transl. (1995). *The Collected Papers of Albert Einstein*. Vol. 5. *The Swiss Years: Correspondence, 1902–1914*. Princeton: Princeton University Press.
- Bohr, Niels. (1923 [1922]). “The structure of the atom.” *Nature* **112**, 1–16 [Nobel Lecture, December 11, 1922]. In Nobel Foundation (1965), pp. 7–43. In Nielsen (1977), pp. 467–482.
- Bohr, N., Kramers, H.A., and Slater, J.C. (1924). “The Quantum Theory of Radiation.” *Philosophical Magazine* **97**, 785–802. In Stolzenburg (1984), pp. 101–118.
- Bothe, W. and Geiger, H. (1925a). “Experimentelles zur Theorie von Bohr, Kramers und Slater.” *Die Naturwissenschaften* **13**, 440–441.
- Bothe, W. and Geiger, H. (1925b). “Über das Wesen des Comptoneffekts: ein experimenteller Beitrag zur Theorie der Strahlung.” *Zeitschrift für Physik* **32**, 639–663.
- Bridgman, P.W. (1936). “Biographical Memoir of William Duane 1872–1935.” *National Academy of Sciences Biographical Memoirs* **18**, 23–41.
- Buchwald, Jed Z. (1994). *The Creation of Scientific Effect: Heinrich Hertz and Electric Waves*. Chicago: University of Chicago Press.

---

<sup>35</sup>Bohr, Kramers, and Slater (1924).

<sup>36</sup>Ellis (1926).

<sup>37</sup>Bothe and Geiger (1925a, 1925b).

<sup>38</sup>Bohr to Fowler, April 21, 1925. In Stolzenburg (1984), pp. 81–84; quote on p. 82.

<sup>39</sup>Einstein to Ehrenfest, August 18, 1925. Quoted in Klein (1970), p. 35.

- Compton, Arthur H. (1922). "Secondary Radiations produced by X-Rays, and Some of their Applications to Physical Problems," *Bulletin of the National Research Council* **4**, Part 2 (October), 1–56. In Shankland (1973), pp. 321–377
- Compton, Arthur H. (1923a). "A Quantum Theory of the Scattering of X-Rays by Light Elements," *Physical Review* **21**, 483–502. In Shankland (1973), pp. 382–401.
- Compton, Arthur H. (1923b). "The Total Reflexion of X-Rays." *Philosophical Magazine* **45**, 1121–1131. In Shankland (1973), pp. 402–412.
- Compton, Arthur H. (1967). "Personal Reminiscences." In Johnston (1967), pp. 3–52.
- Debye, P. (1923). "Zerstreuung von Röntgenstrahlen und Quantentheorie." *Physikalische Zeitschrift* **24**, 161–166. Translated in Debye (1954), pp. 80–88.
- Debye, P. (1954). *The Collected Papers of Peter J.W. Debye*. New York: Interscience.
- Duncan, Anthony and Janssen, Michel. (2007). "Pascual Jordan's resolution of the conundrum of the wave-particle duality of light." Preprint submitted to Elsevier Science, 53 pp. September 18.
- Einstein, A. (1905). "Über einen die Erzeugung und Verwandlung des Lichtes betreffenden heuristischen Gesichtspunkt." *Annalen der Physik* **17**, 132–148. In Stachel (1989), pp. 150–166; Beck (1989), pp. 86–103.
- Einstein, A. (1909a). "Zum gegenwärtigen Stand des Strahlungsproblems." *Physikalische Zeitschrift* **10**, 185–193. In Stachel (1989), pp. 542–550; Beck (1989), pp. 357–375.
- Einstein, A. (1909b). "Über die Entwicklung unserer Anschauungen über das Wesen und die Konstitution der Strahlung." *Verhandlungen der Deutschen Physikalischen Gesellschaft* **7**, 482–500; *Physikalische Zeitschrift* **10**, 817–826 (with "Discussion"). In Stachel (1989), pp. 564–582, 585–586; Beck (1989), pp. 379–398.
- Ellis, C.D. (1926). "The Light-Quantum Theory." *Nature* **117**, 896.
- Eve, A.S. (1939). *Rutherford: Being the Life and Letters of the Rt Hon. Lord Rutherford, O.M.* New York: Macmillan and Cambridge: Cambridge University Press.
- Friedrich, W., Knipping, P., and Laue, M. (1912). "Interferenz-Erscheinungen bei Röntgenstrahlen." *Bayerische Akademie der Wissenschaften, Sitzungsberichte*, 303–322. In Laue (1961), pp. 183–207.
- Hoffmann, Banesh (1972). *Albert Einstein: Creator and Rebel*. New York: The Viking Press.
- Jenkin, John (2002). "G.E.M. Jauncey and the Compton Effect." *Physics in Perspective* **2**, 320–332.
- Johnston, Marjorie, ed. (1967). *The Cosmos of Arthur Holly Compton*. New York: Alfred A. Knopf.

- Kargon, Robert H. (1982) *The Rise of Robert Millikan: Portrait of a Life in American Science*. Ithaca and London: Cornell University Press.
- Klein, Martin J. (1963). "Einstein's First Paper on Quanta." *The Natural Philosopher* **2**, 57–86.
- Klein, Martin J. (1964). "Einstein and the Wave-Particle Duality." *The Natural Philosopher* **3**, 1–49.
- Klein, Martin J. (1970). "The First Phase of the Bohr-Einstein Dialogue." *Historical Studies in the Physical Sciences* **2**, 1–39.
- Klein, Martin J., Kox, A.J., and Schulmann, Robert, ed. (1993). *The Collected Papers of Albert Einstein*. Vol. 5. *The Swiss Years: Correspondence, 1902–1914*. Princeton: Princeton University Press.
- Kuhn, T.S. and Uhlenbeck, G.E. (1962). Interview with Peter Debye, Archive for the History of Quantum Physics, May 3.
- Laue, M. (1912). "Eine quantitative Prüfung der Theorie für die Interferenz-Erscheinungen bei Röntgenstrahlen." *Bayerische Akademie der Wissenschaften, Sitzungsberichte*, 363–373. In Laue (1961), pp. 208–218.
- Laue, Max von (1961). *Gesammelte Schriften und Vorträge*. Band I. Braunschweig: Friedr. Vieweg & Sohn.
- Lenard, P. (1902). "Über die lichtelektrische Wirkung." *Annalen der Physik* **8**, 149–198. In Lenard (1944), pp. 251–290.
- Lenard, P. (1944). *Wissenschaftliche Abhandlungen*. Band 3. *Kathodenstrahlen, Elektronen, Wirkungen Ultravioletter Lichtes*. Leipzig: Verlag von S. Hirzel.
- Millikan, R.A. (1916). "A Direct Photoelectric Determination of Planck's 'h'." *Physical Review* **7**, 355–388.
- Millikan, Robert Andrews. (1917). *The Electron: Its Isolation and Measurement and the Determination of Some of its Properties*. Chicago: University of Chicago Press.
- Millikan, Robert A. (1950). *The Autobiography of Robert A. Millikan*. New York: Prentice-Hall.
- Millikan, Robert Andrews and Gale, Henry Gordon (1906). *A First Course in Physics*. Boston: Ginn & Company.
- Nielsen, J. Rud, ed. (1976). *Niels Bohr Collected Works*. Vol. 3. *The Correspondence Principle (1918–1923)*. Amsterdam: North-Holland.
- Nielsen, J. Rud, ed. (1977). *Niels Bohr Collected Works*. Vol. 4. *The Periodic System (1920–1923)*. Amsterdam: North-Holland.
- Nobel Foundation. (1965). *Nobel Lectures including Presentation Speeches and Laureates' Biographies: Physics 1922–1941*. Amsterdam: Elsevier.

## Einstein's Revolutionary Light-Quantum Hypothesis

---

- Shankland, Robert S., ed. (1973). *Scientific Papers of Arthur Holly Compton: X-Ray and Other Studies*. Chicago: University of Chicago Press.
- Stachel, John, ed. (1989). *The Collected Papers of Albert Einstein*. Vol. 2. *The Swiss Years: Writings, 1900–1909*. Princeton: Princeton University Press.
- Stolzenburg, Klaus, ed. (1984). *Niels Bohr Collected Works*. Vol. 5. *The Emergence of Quantum Mechanics (Mainly 1924–1926)*. Amsterdam: North-Holland.
- Stuewer, Roger H. (1971). “Hertz’s Discovery of the Photoelectric Effect.” *Proceedings of the XIIIth International Congress in the History of Science*, Section VI. Moscow, pp. 35–43.
- Stuewer, Roger H. (1975). *The Compton Effect: Turning Point in Physics*. New York: Science History Publications.
- Thomson, George Paget (1964). *J.J. Thomson and the Cavendish Laboratory in his Day*. London: Nelson.



## 2 The Odd Couple: Boltzmann, Planck and the Application of Statistics to Physics (1900–1913)

MASSIMILIANO BADINO

*In the last forty years a vast scholarship has been dedicated to the reconstruction of Planck's theory of black-body radiation and to the historical meaning of the quantization. Since the introduction of quanta took place for combinatorial reasons, Planck's understanding of statistics must have played an important role. In the first part of this paper, I sum up the main theses concerning the status of the quantum and compare the arguments supporting them. In the second part, I investigate Planck's usage of statistical methods and the relation to Boltzmann's analogous procedure. I will argue that this way of attacking the problem is able to give us some interesting insights both on the theses stated by the historians and on the general meaning of Planck's theory.*

### A Vexed Problem

In his epoch-making paper of December 1900 on the black-body radiation,<sup>1</sup> for the first time Max Planck made use of combinatorial arguments. Although it was a difficult step to take, a real “act of desperation” as he would call it later, Planck pondered it deeply and never regretted it. As he wrote to Laue on 22 March 1934: “My maxim is always this: consider every step carefully in advance, but then, if you believe you can take responsibility for it, let nothing stop you.”<sup>2</sup>

The difficulty involved in this step was the adoption of a way of reasoning Planck had been opposing for a long time: Ludwig Boltzmann's statistical approach. But, even after accepting the necessity of introducing statistical considerations into radiation theory, the application of Boltzmann's theory of complexions to the particular problem of finding the spectral distribution of the cavity radiation was not a straightforward one. In fact, the final result seems to bear only a partial resemblance to Boltzmann's original arguments and the opinions of the scholars are split about the correct interpretation of the relation between Planck's and Boltzmann's statistical procedure. The importance of the issue is enhanced by the fact that, in the secondary literature, close relations can be found with the problem of continuity or discontinuity of energy, i.e. whether Planck conceived the quantization of energy as something real or merely as a computational device. With unavoidable simplifications, we can divide the positions about the historical problem of quantization into three main categories: discontinuity thesis, continuity thesis and weak

---

<sup>1</sup>(Planck, 1900b); (Planck, 1958), 698–706.

<sup>2</sup>Quoted in (Heilbron, 1986, p. 5).

thesis. First, we have the discontinuity thesis according to which Planck worked with discrete elements of energy. As early as 1962, Martin Klein, in a series of seminal papers on this historical period,<sup>3</sup> argued along this direction claiming more or less explicitly that in December 1900 Planck introduced the quantization of energy even though he might have not been perfectly aware of the consequences of this step. Furthermore, in recent years, Res Jost has polemically endorsed Klein's classical thesis against the most distinguished upholder of the continuity thesis, namely Thomas Kuhn.<sup>4</sup>

Indeed, in 1978, Thomas Kuhn<sup>5</sup> claimed that in December 1900, and at least until 1908, Planck was thinking in terms of continuous energy and that his energy elements were merely a shortcut to talk of a continuous distribution over energy cells. The discontinuity entered physics as late as 1905–1906 through the work of Paul Ehrenfest and Albert Einstein. I will call this claim the continuity thesis. Both the discontinuity and the continuity thesis argue for a definite commitment of Planck's on the issue of quantization. In a sense also Olivier Darrigol<sup>6</sup> can be numbered among the upholders of this thesis, even though his position points less straightforwardly towards a clear commitment and it is halfway between continuity and the third option, the weak thesis.<sup>7</sup>

As a matter of fact, the advocates of the weak thesis claim that we cannot single out any clear-cut position of Planck's on the issue of the reality or the physical significance of quantization. The reasons and the meaning of this absence of decision might be different. Allan Needell, for instance, has convincingly argued that this issue was simply out of the range of Planck's interests.<sup>8</sup> The exact behaviour of the resonator belongs to a domain of phenomena, namely the micro-phenomena, Planck was unwilling to tackle from the very beginning of his research program. Hence, the question whether the resonator really absorbs and emits quanta of energy was irrelevant in Planck's general approach. Much more important to understand his theory, Needell suggests, is to look at the role played by the absolute interpretation of the second law of thermodynamics.

A similar contention was shared by Peter Galison who maintains that, in general, it is not wise to ascribe strong commitments to scientists working in a period of scientific crisis.<sup>9</sup> Recently, Clayton Gearhart<sup>10</sup> has suggested another option for the supporters of the weak thesis, holding that even if Planck might have been interested in the issue of the quantization of energy, for various reasons he was unable or unwilling to take a plain position on the status of the energy elements in his printed writings while "he was often more open in discussing their implication in his correspondence."<sup>11</sup> His papers in the crucial period 1900–1913 show an incessant shift and change of emphasis between continuity and discontinuity so that both a literal interpretation (the starting point of Klein's thesis) and a re-interpretation (the main tool of Kuhn's approach) of these papers wind up to be misleading. For Gearhart what Planck lacked was not the interest

---

<sup>3</sup>(Klein, 1962); (Klein, 1963a); (Klein, 1963b); (Klein, 1964); (Klein, 1966). The original source of the discontinuity thesis is (Rosenfeld, 1936).

<sup>4</sup>(Jost, 1995); see also (Koch, 1991).

<sup>5</sup>(Kuhn, 1978) and (Kuhn, 1984). See also (Klein, Shimony, & Pinch, 1979).

<sup>6</sup>(Darrigol, 1988) and (Darrigol, 1991).

<sup>7</sup>Darrigol's position is wholly presented in his recent papers (Darrigol, 2000) and (Darrigol, 2001).

<sup>8</sup>(Needell, 1980).

<sup>9</sup>(Galison, 1981).

<sup>10</sup>(Gearhart, 2002). (Kangro, 1970) holds a weak thesis on Planck's commitment as well.

<sup>11</sup>(Gearhart, 2002, p. 192).

in the issue of quantization (which is testified by his letters and by his trying different approaches), but rather a concluding argument to make up his mind in a way or in another. Also Elisabeth Garber argued in the direction of a certain ambiguity in Planck's work when she claimed that his theory was perceived as escaping the pivotal point: the mechanism of interaction between matter and radiation.<sup>12</sup>

In this debate, a central role is played by the statistical arguments and, notably, by the comparison between Planck's usage of them and Boltzmann's original doctrine because, in effect, the statistical procedure is the first and the main step in Planck's theory where any discontinuity is demanded. Literally interpreted, Planck's statements in December 1900 and in many of the following papers seem to suggest a counting procedure and a general argument that strongly differ from Boltzmann's, pointing to the direction of real and discontinuous energy elements. In fact, one of Klein's main arguments consists in showing how remarkably Planck's use of combinatorials diverges from Boltzmann's and this makes sensible to think that the physical interpretations behind them must diverge as well.<sup>13</sup>

On the contrary, both Kuhn and Darrigol endeavoured to show that the dissimilarities are only superficial or irrelevant. In particular, Kuhn argued that Planck's counting procedure with energy elements is perfectly consistent with Boltzmann's interpretation based on energy cells and that all we need is not to take Planck's statements too literally, but to see them in the historical context of his research program. A discontinuous view of the energy was too drastic a step to be justified by a statistical argument only.

Therefore, both the advocates of the continuity and those of the discontinuity thesis see an intimate connection between Planck's usage of statistical arguments and the issue of the quantization of energy. Nevertheless, Kuhn started from the ambiguity of Planck's combinatorics to claim a commitment on the issue of quantization and this seemed incorrect to the eyes of the advocates of the weak thesis. If it is true that Planck's statistical arguments can be interpreted as not differing from Boltzmann's as much as they seem to do at first sight, then this duality might rather support the thesis of an absence of commitment in the problem of the reality of the quantum. Thus, even after having ascertained whether or not Planck's statistics differ from Boltzmann's, we have to look at the problem from a broader perspective and establish the role that the alleged similarity or dissimilarity might have played in Planck's theory.

As we have seen, Needell suggested that this broader perspective should encompass Planck's view of the laws of thermodynamics, while Gearhart claims that it should take into account the endless shift of emphasis in the printed writings. However, this approach is not decisive as well, because the analysis of the long-term development of Planck's program was among the most original contributions of the advocates of the continuity strong thesis and one of their most effective sources of arguments.<sup>14</sup> In this paper, I will attempt to investigate the way in which Planck tries to justify the introduction of statistical considerations into physics and to compare it with the analogous attempt pursued by Boltzmann. I think that this strategy is able to retrieve a historical perspective on a crucial problem somehow implicit in the previous discussion: what was Planck's attitude towards the relation between statistics and physical knowledge? Put in other

---

<sup>12</sup>(Garber, 1976).

<sup>13</sup>See in particular (Klein, 1962).

<sup>14</sup>For a recent contribution in this direction see (Büttner, Renn, & Schemmel, 2003).



terms: Did Planck think that the statistical approach is another equally correct way of studying macro- and micro-phenomena as the usual dynamic approach? Of course, an answer to this question requires not only an assessment of the similarities or dissimilarities between Planck's and Boltzmann's statistical formalism, but also a clarification of the general status of this formalism in Planck and Boltzmann and the way in which it was related with the rest of the physical knowledge of electromagnetism (in the first case) and mechanics (in the second case).

In the next sections I will attempt to answer to these questions. My main point is that a close investigation of the role of statistics offers a new and original perspective on the debate mentioned above. In particular, I will claim a sort of intermediate position between continuity and weak thesis. My argument to arrive at this conclusion is twofold. I first will analyze Boltzmann's and Planck's combinatorics focussing especially on the counting procedure, on the issue of the maximization and on the problem of the non-vanishing magnitude of the phase space cell. I will argue that, in all these instances, Planck tries to build up his statistical model remaining as close as possible to Boltzmann's original papers, but that the incompleteness of his analogy brings about some formal ambiguities that are (part of) the cause of his wavering and uncommitted position. At any rate, the deviations from Boltzmann's procedure were generally due (or understood as due) to the particularities of the physical problem Planck was dealing with. Next, I will present a sketchy comparison of Planck's and Boltzmann's justification of the introduction of statistical considerations in physics and I will claim that, in this particular aspect, the opinions of the two physicists differ remarkably. This will suggest us an unexpected twist which will bring us to the final conclusion.

## How the Story Began

There are two different statistical arguments in Boltzmann's works. The first is presented in the second part of his 1868 paper entitled "Studien über das Gleichgewicht der lebendigen Kraft zwischen bewegten materiellen Punkten" and devoted to the derivation of Maxwell's distribution law.<sup>15</sup> This argument, as we will see soon, is extremely interesting both for its intrinsic features and for the investigation of Planck's combinatorics that follows.<sup>16</sup>

In this argument, Boltzmann presupposes that the system is in thermal equilibrium and arrives at an explicit form of Maxwell's equilibrium distribution through the calculation of the marginal probability that a molecule is allocated into a certain energy cell. Let us suppose a system of  $n$  molecules whose total energy  $E$  is divided in  $p$  equal elements  $\epsilon$ , so that  $E = p\epsilon$ . This allows us to define  $p$  possible energy cells  $[0, \epsilon]$ ,  $[\epsilon, 2\epsilon]$ ,  $\dots$ ,  $[(p-1)\epsilon, p\epsilon]$ , so that if a molecule is allocated in the  $i$ -th cell, then its energy lies between  $(i-1)\epsilon$  and  $i\epsilon$ . The marginal probability that the energy of a molecule is allocated in the  $i$ -th cell is given by the ratio between the total number of ways of distributing the remaining  $n-1$  molecules over the cells defined by the total energy  $(p-i)\epsilon$  and the total number of ways of distributing all the molecules. In other words, the marginal probability is proportional to the total number of what in 1877 would be

---

<sup>15</sup>(Boltzmann, 1868); (Boltzmann, 1909, pp. I, 49–96).

<sup>16</sup>An excellent discussion of this section of Boltzmann's paper—that, however, does not include an analysis of the combinatorial part of the argument—can be found in (Uffink, 2007, pp. 955–958).

called “complexions” calculated on an opportunely defined new subsystem of molecules and total energy.<sup>17</sup> This is tantamount to saying that the exact distribution of the remaining molecules is marginalised.

To clarify his procedure, Boltzmann presents some simple cases with a small number of molecules. Let us consider, for instance, the case  $n = 3$ . Boltzmann estimates the total number of ways of distributing 3 molecules over the  $p$  cells by noticing that if a molecule is in the cell with energy  $p\epsilon$ , there is only one way of distributing the remaining molecules, namely in the cell with energy  $0\epsilon$ , if a molecule has energy  $(p - 1)\epsilon$  there are two different ways and so on.<sup>18</sup> Therefore, the total number of ways of distributing the molecules is:

$$1 + 2 + \dots + p = \frac{p(p + 1)}{2}.$$

Now, let us focus on a specific molecule. If that molecule has energy  $i\epsilon$ , then there is  $(p - i)\epsilon = q\epsilon$  energy available for the remaining molecules and this means  $q$  possible energy cells. There are, of course,  $q$  equiprobable ways of distributing 2 molecules over these  $q$  cells because once a molecule is allocated, the allocation of the other is immediately fixed by the energy conservation constraint. Hence, the marginal probability that the energy of a molecule lies in the  $i$ -th cell is:

$$P_i = 2 \frac{q}{p(p + 1)}.$$

With a completely analogous reasoning one can easily find the result for  $n = 4$ :

$$P_i = 3 \frac{q(q + 1)}{p(p + 1)(p + 2)}.$$

Thus, it is clear that, by iterating the argument, in the general case of  $n$  molecules this probability becomes:<sup>19</sup>

$$P_i = (n - 1) \frac{q(q + 1) \dots (q + n - 3)}{p(p + 1) \dots (p + n - 2)}.$$

Letting the numbers of elements and of molecules grow to infinite, Boltzmann obtains the Maxwell distribution.

Some quick remarks regarding this statistical argument. First, the marginalization procedure leads Boltzmann to express the probability that a certain energy is ascribed to a given molecule in terms of the total number of complexions (for a suitable subsystem) and this procedure is closely related to Boltzmann’s physical task: finding the equilibrium distribution. I will return on this point later on. Second, Boltzmann defines the energy cells using a lower and upper limit, but in his combinatorial calculation he considers one value of the energy only. This is doubtless due to the arbitrary small

---

<sup>17</sup>A complexion is a distribution of distinguishable statistical objects over distinguishable statistical predicates, namely it is an individual configuration vector describing the exact state of the statistical model.

<sup>18</sup>Note that, since Boltzmann is working with energy cells, the order of the molecules within the cell is immaterial.

<sup>19</sup>The dependence on  $i$  is contained in  $q$  through the relation  $p - i = q$ .

magnitude of  $\epsilon$ , but it also entails an ambiguity in the passage from the physical case to its combinatorial representation and vice-versa. Third, a simple calculation shows that:

$$\begin{aligned}
 (n-1) \frac{q(q+1) \dots (q+n-3)}{p(p+1) \dots (p+n-2)} &= \frac{(n-1)!}{(n-2)!} \\
 &\times \frac{1 \cdot 2 \cdot \dots \cdot (q-1)q(q+1) \dots (q+n-3)}{1 \cdot 2 \cdot \dots \cdot (q-1)} \\
 &\times \frac{1 \cdot 2 \cdot \dots \cdot (p-1)}{1 \cdot 2 \cdot \dots \cdot (p-1)p(p+1) \dots (p+n-2)} \\
 &= \frac{\binom{q+n-3}{q-1}}{\binom{p+n-2}{p-1}}. \quad (1)
 \end{aligned}$$

It is worthwhile noticing that the distribution (1) is a particular case of the so-called Polya bivariate distribution at that time still unknown.<sup>20</sup> Moreover, the normalization factor in equation (1), i.e. the binomial coefficient at the denominator on the right-hand side, is of course the total number of complexions given the energy conservation constraint as Boltzmann's statistical model suggests. In fact, let us suppose that there are  $n$  distinguishable statistical objects and  $p$  distinguishable statistical predicates, and suppose that to each predicate a multiplicity  $i$  ( $i = 0, \dots, p-1$ ) is ascribed. An individual description that allocates individual objects over individual predicates is valid if and only if:

$$\sum_i in_i = p - 1,$$

where  $n_i$  is the number of objects associated with the predicate of multiplicity  $i$ . Under these conditions, the number  $W$  of valid individual descriptions is:

$$W = \binom{p+n-2}{p-1} = \frac{(p+n-2)!}{(p-1)!(n-1)!}, \quad (2)$$

namely the normalization factor written by Boltzmann. We will meet this formula again in Boltzmann's 1877 paper and, more importantly, this particular form of the normalization factor will play a major role in explaining some ambiguities of Planck's own statistics.

In 1877 Boltzmann devoted a whole paper to a brand new combinatorial argument which presumably constituted Planck's main source of statistical insights.<sup>21</sup> There are notable differences between this argument and its 1868 predecessor, starting with the physical problem: in 1877 Boltzmann is facing the issue of irreversibility and his task is not simply to derive the equilibrium distribution, but to show the relation between this distribution and that of an arbitrary state. Thus Boltzmann replaces the marginalization with a maximization procedure to fit his statistical analysis to the particular physical problem he is tackling.

To substantiate his new procedure, Boltzmann puts forward the famous urn model. Let us suppose, as before, a system of  $n$  molecules and that the total energy is divided into elements  $E = p\epsilon$  and imagine a urn with very many tickets. On each ticket a number

<sup>20</sup>See (Costantini, Garibaldi, & Penco, 1996) and (Costantini & Garibaldi, 1997).

<sup>21</sup>(Boltzmann, 1877); (Boltzmann, 1909, pp. II, 164–223).

between 0 and  $p$  is written, so that a possible complexion describing an arbitrary state of the system is a sequence of  $n$  drawings where the  $i$ -th drawn ticket carries the number of elements to be ascribed to the  $i$ -th molecule. Of course, a complexion resulting from such a process could not possibly satisfy the energy conservation, therefore Boltzmann demands an enormous number of drawings and then eliminates all the complexions that violate the constraint. The number of acceptable complexions obtained by this procedure still is very large. Since a state distribution depends on how many molecules (and not which ones) are to be found in each cell, many different complexions might be equivalent to a single state and Boltzmann's crucial step is to ascribe a probability to each state in term of the number of complexions corresponding to it. By maximizing the state probability so defined, Boltzmann succeeds in showing that the equilibrium state has a probability overwhelmingly larger than any other possible distribution or that there are far more complexions matching the equilibrium state.

Besides the differences in the general structure of the argument, it is worthwhile noting that in this new statistical model Boltzmann must count again the total number of complexions that are consistent with the energy conservation constraint. To do so he uses the formula (2), but in this particular case the possible allocations of energy are  $p + 1$  because the energy cell is defined by a single number of elements rather than by lower and upper limits. This means that the normalization factor (2) becomes:

$$\binom{p+n-1}{p} = \frac{(p+n-1)!}{p!(n-1)!}. \quad (3)$$

This is the total number of complexions for a statistical model where distinguishable objects are distributed over distinguishable predicates precisely as in 1868. Boltzmann actually writes the formula (3) in passing as an expression of the total number of such complexions.<sup>22</sup> However, it can also be interpreted in a completely different way. It can equally well express the total number of occupation vectors for a statistical model of  $p$  indistinguishable objects and  $n$  distinguishable predicates. To put it differently, if one wants to calculate the total number of ways of distributing  $p$  objects over  $n$  predicates counting only how many objects, and not which ones, are ascribed to each predicate, then the formula (3) gives the total number of such distributions. An ingenious and particularly simple way of proving this statement was proposed by Ehrenfest and Kamerlingh Onnes in 1915.<sup>23</sup> Let us suppose that, instead of  $n$  distinguishable cells, one has  $n - 1$  indistinguishable bars defining the cells.<sup>24</sup> If both the  $p$  objects and the  $n - 1$  bars were distinguishable, the total number of individual descriptions would be given by  $(p + n - 1)!$ . But the indistinguishability forces us to cancel out from this number the  $p!$  permutations of the indistinguishable objects and the  $(n - 1)!$  permutations of the indistinguishable bars. By doing so, one arrives at the total number  $W_{ov}$  of occupation vectors:

$$W_{ov} = \frac{(p+n-1)!}{p!(n-1)!}.$$

This purely formal similarity, as we will see in the next section, is one of the keys to understand the ambiguities of Planck's statistical arguments.

<sup>22</sup>(Boltzmann, 1877, pp. II, 181).

<sup>23</sup>(Ehrenfest & Kamerlingh Onnes, 1915).

<sup>24</sup>Note that this switch between cells and limits is similar to Boltzmann's with the not negligible difference that Boltzmann's cell limits in 1868 are distinguishable.

## A Statistics for All Seasons

Planck's application of Boltzmann's statistics to radiation theory has very far-reaching consequences which puzzled his contemporaries and which took many years to be completely understood. In this and in the next section I will restrict myself to some problems that have a special bearing on the historical issue of the quantization, namely the analysis of Planck's counting procedure and the general structure of his statistical argument.

In his December 1900 paper, where he first gives a theoretical justification of the radiation law, Planck is apparently very explicit about his counting procedure:

We must now give the distribution of the energy over the separate resonators of each [frequency], first of all the distribution of the energy  $E$  over the  $N$  resonators of frequency  $\nu$ . If  $E$  is considered to be a continuously divisible quantity, this distribution is possible in infinitely many ways. We consider, however—this is the most essential point of the whole calculation— $E$  to be composed of a well-defined number of equal parts and use thereto the constant of nature  $h = 6.55 \times 10^{-27}$  erg sec. This constant multiplied by the common frequency  $\nu$  of the resonators gives us the energy element  $\epsilon$  in erg, and dividing  $E$  by  $\epsilon$  we get the number  $P$  of energy elements which must be divided over the  $N$  resonators. If the ratio thus calculated is not an integer, we take for  $P$  an integer in the neighbourhood. It is clear that the distribution of  $P$  energy elements over  $N$  resonators can only take place in a finite, well-defined number of ways.<sup>25</sup>

In this passage Planck is unmistakably speaking of distributing energy elements over resonators.<sup>26</sup> Moreover, in the same paper, Planck writes the total number of ways of this distribution in the following way:

$$\frac{N(N+1)(N+2)\dots(N+P-1)}{1\cdot 2\cdot 3\cdot\dots\cdot P} = \frac{(N+P-1)}{(N-1)!P!}. \quad (4)$$

This is the total number of ways of distributing  $P$  indistinguishable objects over  $N$  distinguishable predicates as Ladislav Natanson would point out in 1911.<sup>27</sup> But, as I said commenting formula (3), it can also be interpreted as the total number of ways of distributing  $N$  distinguishable objects over  $P+1$  distinguishable predicates given the energy conservation constraint, namely exactly the same statistical model Boltzmann had worked out in his 1877 paper. While in the first interpretation the distribution of single energy elements over resonators very naturally suggests that the resonators can absorb and emit energy discontinuously, in the second interpretation of the same formula, the resonators are distributed over energy cells that have a fixed magnitude, but they can be placed *everywhere* within a given cell thus implying that they can absorb or emit continuously. More importantly, if Planck was faithfully following Boltzmann in framing his statistical model, and Boltzmann, as we know, assumed a continuous physics behind

<sup>25</sup>(Planck, 1900b); see (Planck, 1972, p. 40).

<sup>26</sup>However, the final part of the quotation seems to suggest that he is not considering  $P$  to be necessarily an integer. On this point see (Darrigol, 2001).

<sup>27</sup>(Natanson, 1911).

his model, it is extremely plausible that Planck did not feel himself forced to assume any discontinuity as a consequence of his counting procedure.<sup>28</sup>

Therefore, the formal ambiguity in Planck's way of counting the complexions deprives of cogency one of the fundamental arguments of the advocates of the discontinuity thesis which relies on the original statement in December 1900. This point can be strengthened by appealing to Planck's awareness of this ambiguity. In the fourth chapter of the first edition of the *Vorlesungen über Wärmestrahlung* (1906), his attempt at remaining as close as possible to Boltzmann's original argument and phraseology is patent. First, Planck introduces the concepts of complexion and distribution for a gas and it is clear that, to him, a complexion is an individual allocation of molecules to energy cells.<sup>29</sup> Then he simply extends this concept to radiation theory, without any, even slight, change of meaning so that it is plausible that this concept keeps its general features in the new context as well.

After developing Boltzmann's procedure for a gas, he deals with the problem of counting complexions in radiation theory:

Here we can proceed in a way quite analogous to the case of gas, if only we take into account the following difference: a given state of the system of resonators, instead of determining a unique distribution, allows a great number of distributions since the number of resonators that carry a given amount of energy (better: that fall into a given 'energy domain') is not given in advance, it is variable. If we consider now every possible distribution of energy and calculate for each one of these the corresponding number of complexions exactly as in the case of gas molecules, through addition of all the resulting number of complexions we get the desired probability  $W$  of a given physical state.<sup>30</sup>

The reference to the "energy domain" clarifies that Planck is thinking of distributing resonators over energy cells and that he considers this way of doing as "a way quite analogous to the case of gas."

But immediately after, he stresses that the same goal can be accomplished by the "faster and easier" ("schneller und bequemer") way of distributing  $P$  energy elements over  $N$  resonators and then he displays again the same formula used in December 1900. This passage shows two important points. First, in 1906 Planck was well aware that, from a purely formal viewpoint, both statistical models led to the same result. Second, he also knew that the distribution of individual energy elements over resonators was a simpler way of doing because it does not require any energy conservation constraint and, more importantly, no assumption on the distribution of the resonators within the energy cells is needed. Unfortunately, this is the first occasion in which Planck explicitly reveals his knowledge of the subtleties of combinatorics and the objection can be made that this knowledge was the fruit of the intervening years between 1900 and 1906. However, it seems unlikely that Planck was not aware of such a trivial equivalence already in December 1900 because the decision of adopting combinatorial considerations was probably

---

<sup>28</sup>This ambiguity was exploited in the other direction by Alexander Bach who in (Bach, 1990) suggested that in 1877 Boltzmann was anticipating a Bose-Einstein statistics. However, I think that Bach's interpretation, though formally correct, cannot be held from a historical point of view.

<sup>29</sup>(Planck, 1906, pp. 140–143).

<sup>30</sup>(Planck, 1906, pp. 151–152).

well pondered by him. Furthermore, the discontinuity thesis loses footing because, as Kuhn pointed out, it is difficult to figure out why Planck, after committing himself to discontinuous emission and absorption in 1900, should have availed himself of a formal equivalence with a combinatorial procedure which presupposes continuous energy cells in 1906.

Further support to the thesis that Planck interpreted the elements of energy in analogy with Boltzmann's procedure is provided by the third lecture delivered by Planck at Columbia University in 1909. The main claim of that lecture is that "irreversibility leads of necessity to atomistics,"<sup>31</sup> precisely because an atomistic hypothesis is an inescapable prerequisite of the application of probability. But, and this is the point, the only role actively played by the atomistic hypothesis consists of allowing us to distinguish the possible cases that are to be computed. Of course, a combinatorial calculation calls for a separation of the various possibilities and this is manifestly unattainable in case of a continuum, hence:

[I]n order to be able to differentiate completely from one another the complexions realizing [a state], and to associate it with a definite reckonable number, there is obviously no other means than to regard it as made up of numerous discrete homogeneous elements—for in perfectly continuous systems there exist no reckonable elements—and hereby the atomistic view is made a fundamental requirement.<sup>32</sup>

Thus Planck conceives the discontinuous elements of energy in the same way as Boltzmann in 1868 and in 1877, namely as formal devices suitable for labelling and then combinatorially manipulating the different cases and, of course, this function can be equally well accomplished by energy cells. Therefore, the formal similarity, Planck's awareness of it and his interpretation of the 'elements' seem to suggest powerfully that he did not perceive any fracture between his theory and classical physics.

On the other hand, the continuity thesis is not so compelling as it can appear at first sight, at least as far as its most ambitious conclusions are concerned. In fact, Planck's 1906 awareness of the formal similarity mentioned above does not straightforwardly support Kuhn's claim that he was committed to a continuous physical model. This inference is possible only after admitting a close interplay between statistics and physics in Planck's theory, otherwise the formal similarity turns out to be nothing but a formal ambiguity and Planck's awareness reduces itself to the possibility of maintaining an uncommitted position, precisely the content of the weak thesis. Such an interplay was typical of Boltzmann's style but, I will argue, absolutely absent in Planck's. Of course, it might be claimed that continuity in the energy exchange between resonators and field would have been much more attractive to Planck than a discontinuity which seemed to entail a contradiction with Maxwell's equations. However, this appeal to Planck's theoretical background is not conclusive because, as Allan Needell has persuasively shown, a fundamental ingredient of this background consisted in avoiding any explicit assumption on the microstructure of the system. Indeed, Planck chose the case of the black-body radiation because there was no need of specifying the detailed internal structure of the

---

<sup>31</sup>(Planck, 1915, p. 41).

<sup>32</sup>(Planck, 1915, p. 45).

resonators. Therefore, Planck's research program might be utilized to support both the continuity thesis and the weak thesis.

A problem with Needell's argument is that Planck's statements about his program mainly belongs to a period before the development of his combinatorics, so that a supporter of the continuity thesis might argue that Planck, after his conversion to Boltzmann's combinatorics, abandoned or weakened the neutrality towards the microstructure that characterized the first phase of his program. This objection would shift the problem to another question: when did Planck's conversion actually take place and how deep was it? There is another way to tackle the issue: as I have said above, the continuity thesis heavily relies on the status ascribed by Planck to the statistical arguments and, fortunately enough, there are clear statements about this topic in the first edition of the *Vorlesungen*. But before analysing them, I will complete the survey of Planck's application of Boltzmann's combinatorics discussing the general structure of his statistical argument.

## To Maximize or Not to Maximize?

The first paper on the quantum was published on December 1900 and the second in the *Annalen der Physik* on January 1901.<sup>33</sup> In spite of such a tiny interval of time, there are considerable differences between these two papers, particularly with regard to the structure of the argument.

In the first paper, Planck considers different classes of resonators characterized by their proper frequency of vibration. Thus we have  $N_1$  resonators at frequency  $\nu_1$ ,  $N_2$  resonators at frequency  $\nu_2$ , and so on. All resonators of a certain class have the same frequency and they do not mutually interact. Next Planck supposes that the total energy of the system consisting of resonators and radiation is  $E$ , and  $E_r$  is the fraction of the total energy belonging to the resonators only. The energy  $E_r$  must be divided over the different frequencies, so that a possible energetic state of the system of resonators is described by the vector:

$$\omega_k = \{E_1, E_2, \dots\}, \quad (5)$$

where  $E_i$  is the energy assigned to the frequency  $\nu_i$  and each vector  $\omega_k$  must satisfy the condition:

$$E_r = E_1 + E_2 + \dots$$

There are many different ways of distributing the total energy  $E_r$  over the possible frequencies in accordance with the condition above, but not all these ways have the same 'probability.' Planck suggests to measure the probability that a certain energy  $E_i$  is ascribed to the frequency  $\nu_i$  by the total number of ways of distributing the energy divided in  $P_i$  elements of magnitude  $\epsilon_i = h\nu_i$  over the  $N_i$  resonators. Since the magnitude of the elements depends on the frequency, the division of energy is different in each class of resonators. As we have already seen, this number is:

$$W(E_i) = \frac{(N_i + P_i - 1)}{(N_i - 1)!P_i!}. \quad (6)$$

---

<sup>33</sup>(Planck, 1901).



Since resonators of different classes do not interact, the distribution described by the vector (5) is a compound event consisting of many independent events, then its probability is:

$$W(\omega_k) = \prod_i W(E_i). \quad (7)$$

At this point, instead of performing the cumbersome maximization of (7), finding the equilibrium distribution  $\omega_{eq}$  and the mean energy of a resonator at an arbitrary frequency, Planck mentions that “[a] more general calculation which is performed very simply, using exactly the above prescriptions shows much more directly” the final result. There is no description at all of what this “general calculation” should look like and Thomas Kuhn has suggested that here Planck has in mind the argument he would present in his *Annalen* paper in January 1901. Kuhn’s hypothesis is perfectly reasonable because the only problem with the calculation above is the maximization procedure which actually does not appear in the 1901 paper. Indeed, in the January article Planck starts by reckoning only a class of resonator and does not consider a set of arbitrary distributions  $\omega_k$  among which a particular equilibrium distribution  $\omega_{eq}$  is to be selected by means of a maximization procedure, but he directly presupposes the equilibrium state. After this step, the procedure is similar to the December paper with the calculation of (6) for a single class of resonators and without equation (7). Both arguments present deviations from Boltzmann’s original procedure which have been deeply studied by historians<sup>34</sup> but I think that some confusion still remains as regarding to the justification of such deviations in the context of Planck’s theory.

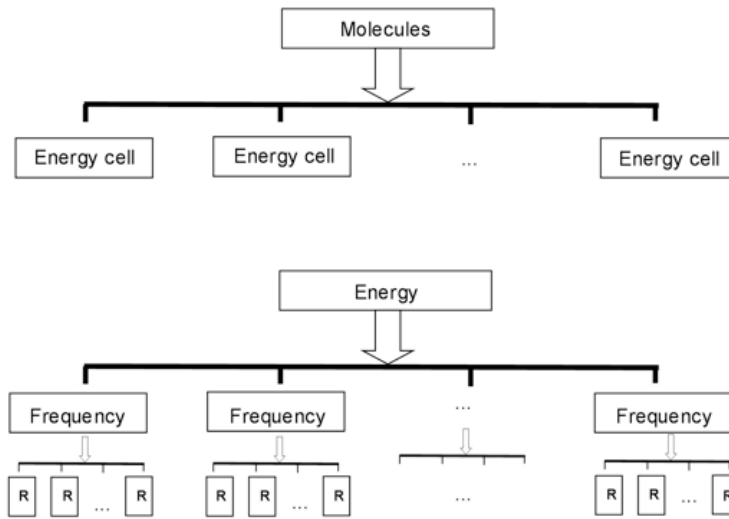
First, it has been stressed that Planck uses the total number of ‘complexions’ (ways of distributing the energy over the resonators of a certain class) instead of the number of complexions consistent with a certain distribution. It is doubtless true that, whichever statistics Planck is using, his calculation involves the total number of ways of distribution, but before deeming it a relevant deviation from Boltzmann’s procedure we must first examine the physical problem Planck is dealing with.

In Boltzmann’s theory a macrostate is given by the number of molecules that are placed in a certain energy interval, a situation that in equilibrium is described by Maxwell’s distribution for a gas. On the contrary, in the case of radiation theory what is physically meaningful is a relation between the energy allocated to a certain frequency and the absolute temperature and this relation presupposes a calculation of the total energy at each frequency. This distribution of energy over frequencies, condensed in (5), is a *macrostate* in Planck’s theory while the distribution of the energy over a class of resonators (how many resonators lie in a certain energy cell) is still a *microstate*.<sup>35</sup> The difference between Boltzmann’s and Planck’s physical situation is outlined by the following scheme:

---

<sup>34</sup>See especially (Klein, 1962), (Kuhn, 1978), (Darrigol, 1988), and (Gearhart, 2002).

<sup>35</sup>On this important difference see also (Darrigol, 2000) and (Darrigol, 2001).



In Boltzmann’s case a microstate is an individual arrangement of molecules over different energy cells, while a macrostate is given by the number of molecules allocated in each cell. Instead, in Planck’s, energy is allocated over each frequency and then divided in elements which are distributed over the resonators (R) that vibrate at that frequency. A microstate is an individual arrangement of resonators in energy cells, while a macrostate is how much energy is allocated to each frequency.

To make this delicate point as clear as possible we can consider where the disanalogy between Planck and Boltzmann stems from. To transform Boltzmann’s case in Planck’s one we can proceed as follows. Let us suppose to have  $N$  molecules, so that a state distribution is a vector:

$$o_k = \{n_0, n_1, \dots, \},$$

quite analogous to vector (5). This vector tells us that  $n_i$  molecules are in the cell with energy  $i$ . Let us now suppose that no permutations are possible among the different energy cells, precisely like no exchange of energy is possible among resonators of different frequency. This also means that one should suppose the molecules as distributed in bunches of dimension  $n_i$  over each cell—as described by the vector  $o_k$ —but not singularly, because otherwise one could obtain the same result as a permutation by distributing individual molecules on different cells alternatively. This is also due to the fact that the elements of energy only make physical sense when they are associated with a certain frequency, hence we can only ascribe energy as a whole to a frequency and then divide it in  $P$  elements, if necessary by taking “for  $P$  an integer in the neighbourhood.” Furthermore, since in Planck’s model there are many resonators at each frequency, we must suppose that each energy cell is divided in a number of sub-levels, so that the molecules can be allocated in different ways within each cell. It is clear that, in this modification of Boltzmann’s model of distributing molecules over energy cells, a macrostate is defined by the vector  $o_k$ , but a microstate is no longer an allocation of individual molecules within the cells (because we cannot speak of individual molecules allocated in the cells), but an allocation of individual molecules over the sub-levels of each cell. In this case, the natural way of defining the probability of a distribution described by the vector  $o_k$  is to make it proportional to the total number of ways of distributing the

molecules over the sub-levels. It is exactly what Planck did and it is actually nothing more than an application of Boltzmann's general rule according to which the probability of a macrostate is proportional to the total number of microstates that leave the macrostate unchanged or that are consistent with that macrostate.

Two comments follow from this model. First, it clearly shows what was really tricky in Planck's usage of statistics. If the molecules have to be distributed in bunches, then it does not make sense to talk of the distribution of a single molecule because there is a sort of statistical correlation between molecules located in the same energy cell. This is exactly the main characteristic of Bose-Einstein statistics. But this crucial point is concealed by the fact that Planck is speaking of energy and his microstate concerns the distribution of resonators.<sup>36</sup> As soon as a corpuscular conception of energy gained a sound footing and the resonators were left aside, the troublesome features of Planck's daring analogy would emerge, because what was a macrostate in Planck immediately became one of many equiprobable microstates and the bunches of energy became groups of indistinguishable particles. Not surprisingly, the first step Albert Einstein took in his 1924 paper on quantum statistics was to reduce Planck's macrostate to the rank of a microstate and to define a new sort of macrostate.<sup>37</sup>

Secondly, however, as long as one keeps assuming the energy as a continuous quantity and using the resonators as a further level of description, the oddities in Planck's model remain hidden. From this point of view, Planck could have considered his usage of statistics as a straightforward application of Boltzmann's doctrine because he ultimately evaluated the probability of a certain macrostate (7) through *the total number of microstates consistent with that macrostate*. The difference from Boltzmann rested mainly on the definition of macrostate, but, in turn, it depended more on the particular physical problem, than on the statistical argument used.<sup>38</sup> Planck is very clear on this topic in the first edition of the *Vorlesungen*:

In this point lies the essential difference between the [radiation theory] case and that of a gas. Since in the latter the state was defined by the space and velocity distribution among the molecules [...]. Only when the distribution law is given, the state can be considered as known. On the contrary, in the former case for the definition of the state suffices the calculation of the total energy  $E$  of the  $N$  resonators; the specific distribution of the energy over the single resonator is not controllable, it is completely left [anheimgegeben] to chance, to elementary disorder.<sup>39</sup>

More subtle is the issue concerning the maximization because it involves Planck's particular concept of disorder. As early as December 1900, Planck notices that the

---

<sup>36</sup>The model also shows that it is statistically irrelevant whether the resonators are distributed over the energy cells or the energy elements are distributed over the resonators. Planck's statistical leap lies elsewhere, and to make it come to light the resonators have to be abandoned.

<sup>37</sup>(Einstein, 1924, p. 262).

<sup>38</sup>It should be noticed in passing that, even in 1877, Boltzmann marginalized the complexions in the position space. In fact, Maxwell's distribution holds for the velocities only, hence a Boltzmann's macrostate is characterized by the product of the number of the favourable complexions in the velocity space and the total number of complexions in the position space. Of course Boltzmann does not consider this number explicitly because it is an unimportant constant. On this point see (Hoyer, 1980).

<sup>39</sup>(Planck, 1906, p. 151); an akin statement can be found in (Planck, 1915, p. 89).

notion of entropy is closely connected to the chaotic feature of the system but, at the same time, the way in which the disorder enters a system of resonators is radically different from the way in which the same concept is applied in gas theory. In the former case, the disorder takes the form of “natural radiation,” a particular assumption on the incoherent variation of the Fourier components of the waves exciting a resonator. This means that, while in a gas the disorder concerns the mutual interaction of very many molecules at a given instant, in radiation theory the disorder is a feature of the interacting field and affects the evolution of a single resonator during a long interval of time. In other words, in a gas the disorder is a characteristic of a set of molecules at a given instant, while in cavity radiation, it is a characteristic of the temporal evolution of individual resonators. It is precisely this shift of meaning that allows Planck to introduce the entropy for a single resonator, a concept that would not make sense in gas theory.

Planck was probably aware of this fundamental difference from the outset because he mentions it in the introduction of his paper in March 1900.<sup>40</sup> However, it is only in the first edition of the *Vorlesungen* that an explicit statement on the influence of this aspect on the combinatorics of the resonators can be found:

Briefly said: in the thermal oscillations of a resonator the disorder is temporal, while in the molecular motion of a gas it is spatial. However, this difference is not so important for the calculation of the entropy of a resonator as it might appear at first sight; because through a simple consideration can be stressed what is essential for a uniform treatment.<sup>41</sup>

The “simple consideration” comes immediately after:

The temporal mean value  $U$  of the energy of a single resonator in an irradiating vacuum is evidently equal to the mean value of the energies calculated for a particular instant over a large number  $N$  of identical resonators that find themselves in the same radiation field but so far away from each other that their oscillations do not influence one another.

These statements clarify an analogous—but more obscure—passage in the December 1900 paper where Planck suddenly leaps from the temporal disorder of a single resonator to the calculation of the distribution of energy over a set of identical resonators without any apparent justification. Obviously Planck was aware of the connection mentioned above already in December 1900. Most probably, Planck’s confidence in the ‘evidence’ of the equivalence—that at first sight is not evident at all!—stems from Boltzmann’s *Gastheorie*. In Section 35 of the second volume, Boltzmann comes up with a qualitative argument to extend the validity of the equipartition theorem proved for a gas to a thermal system in an arbitrary state of aggregation. The presupposition of the argument is a fact of experience: warm bodies reach a stable state of equilibrium. In this state kinetic energy does not differ appreciably from the mean in the course of time. Moreover, this state is independent of the initial conditions, so that Boltzmann can state:

... we can also obtain the same mean values if we imagine that instead of a single warm body an infinite number are present, which are completely

---

<sup>40</sup>(Planck, 1900a); see (Planck, 1958, pp. 668–686).

<sup>41</sup>(Planck, 1906, p. 150).

independent of each other and, each having the same heat content and the same external conditions, have started from all possible initial states. We thus obtain the correct averages values if we consider, instead of a single mechanical system, an infinite number of equivalent systems, which started from arbitrary different initial conditions.<sup>42</sup>

This argument must have pleased Planck very much because it only relies on the thermal equilibrium as an empirical fact and, as a consequence, on the elementary disorder.

In fact, in the December 1900 paper, we find an important hint in this direction that is missing in the *Vorlesungen*. Planck states that a key requirement for adopting his combinatorial derivation is “to extend somewhat the interpretation of the hypothesis of natural ‘radiation’ which has been introduced by me into electromagnetic theory.”<sup>43</sup> The generalization of the hypothesis of natural radiation Planck is talking about is exactly the broader concept of elementary disorder that he considers the foundation of the statistical description of the system. One can represent the temporal evolution of a single resonator by means of the combinatorics over a set of many identical resonators precisely because both models are disordered in the same sense and this concept of disorder is shared with gas theory as well. Therefore, one can apply in radiation theory the combinatorial methods that naturally follow from the notion of disorder in gas theory, because, viewed from a general perspective, there is an analogous notion in radiation theory as well. In other words, the elementary disorder is supposed to bridge the gap between the physical description of a resonator interacting with a field and its combinatorial description as a set of identical copies and to make this leap ‘evident.’ One can replace the former with the latter only if the temporal evolution of the system is disordered in the same sense as a distribution over the copies is.

Indeed, to accomplish his final goal, Planck had to find a relation between the energy  $E_\nu$  allocated on the frequency  $\nu$  and the absolute temperature  $T$ . The entropy  $S$  is a concept connecting both quantities by means of the well-known definition of absolute temperature:

$$\frac{\partial S}{\partial E} = \frac{1}{T}.$$

Adopting Boltzmann’s definition of entropy:

$$S = k \log W,$$

one only needs a relation between the probability  $W$  and the energy  $E$ . In December 1900, Planck writes:

Entropy means disorder, and I thought that one should find this disorder in the irregularity with which even in a completely stationary radiation field the vibrations of the resonator change their amplitude and phase, as long as one considers time intervals long compared to the period of one vibration, but short compared to the duration of a measurement.<sup>44</sup>

---

<sup>42</sup>(Boltzmann, 1898, p. 310).

<sup>43</sup>(Planck, 1900b); see (Planck, 1972, p. 39).

<sup>44</sup>(Planck, 1900b); see (Planck, 1972, p. 38).

Thus, elementary disorder in terms of natural radiation warrants a disordered temporal evolution of the resonator. But Planck still needs, in December 1900, a *measure* of this disorder, a quantitative expression of the disorder involved in the fact that the energy  $E$  is allocated on the (resonator of) frequency  $\nu$ .<sup>45</sup> This measure, namely the probability  $W$ , is provided by the combinatorics on the system of  $N$  identical resonators, but the foundation of this bold leap is the general notion of elementary disorder.

In the meantime, another ambiguity jumps out of the hat. On the one hand, Planck's analysis of the statistical model fits Boltzmann's procedure in seeking for an equilibrium distribution among the possible ways of allocating energy over the frequencies. On the other hand, if the single resonator is in equilibrium with the field during the long time considered, then the statistical model of  $N$  resonators must represent a state of equilibrium as well. If the temporal behaviour of a single resonator in equilibrium is equal to the combinatorial behaviour of a set of resonators as regards the average values, then all the configurations calculated in the set must represent equilibrium configurations.<sup>46</sup> From this point of view, a maximization procedure is conceptually unnecessary because all the ways of distributing the energy elements over the resonators are consistent with the equilibrium state. By using the fact that his physical problem (the derivation of the black-body radiation law) is defined for the equilibrium state only and by a daring application of the elementary disorder, Planck can escape the formal necessity of maximization. In fact, such a procedure is relevant only if one is interested in the problem of irreversibility but, as we will see more clearly below, Planck considers this issue completely solved by the notion of elementary disorder and, from 1900 on, it disappears from his research program. With the riddle of irreversibility put aside, the only problem remaining was the derivation of the radiation law.

For these reasons, Planck was free to use the maximization or not without affecting the consistency of his reasoning or the analogy with Boltzmann's statistical arguments and he seems to be aware of this since December 1900. Furthermore, as we have seen, Boltzmann himself, in 1868, elaborated a statistical argument dealing with the equilibrium state only, which did not make use of the maximization procedure, a technique that would make its appearance only in 1877, in close connection with the problem of irreversibility. Unsurprisingly, given the chance, Planck chose the "faster and easier" way of avoiding maximization.

### Size Does Matter

A further departure of Planck's statistics from Boltzmann's is the fixed magnitude of the energy element. Boltzmann divided the energy space into cells, but the magnitude of these cells was completely arbitrary and disappeared from the final result. By contrast, the magnitude of Planck's elementary cells (*Elementargebiete*) was determined by a universal constant that played a crucial role in the final formula. Once again, Planck

---

<sup>45</sup>As pointed out by Needell, Planck considered probability merely (or mainly) as a measure of disorder and, indirectly, as a way for calculating entropy. This is clear, for instance, in (Planck, 1901) where he says that the combinatorial definition of probability is "the condition [...] which permits the calculation of  $S$ ," see (Planck, 1958, p. 719).

<sup>46</sup>Note that the temporal evolution of a resonator is analogous to a system in thermal contact with a heat reservoir. In both cases the exact energy of the system can fluctuate around a mean even though the equilibrium is maintained. On this point see also (Gearhart, 2002).

was conscious of this fact that, in the *Vorlesungen*, he considers “an essential difference” with the case of gas.<sup>47</sup> He also knew that if the magnitude of the elementary cell goes to zero, one retrieves the incorrect Rayleigh-Jeans formula.<sup>48</sup>

But even if it was an essential difference in the procedure, Planck tried to assign to the unvanishing size of the cell a place in the framework of the combinatorial approach. In December 1900, the division of the energy in elements of fixed magnitude was performed to allow the combinatorial calculation and the choice of the constant  $h$  was probably due to the law Planck had found in October.<sup>49</sup> However, in the first edition of the *Vorlesungen*, Planck discovers an important meaning of the universal constant. He shows that  $h$  can be interpreted as the elementary area, i.e. area of equal probability, in the phase space of the resonator.

This interpretation actually strengthens the link with Boltzmann for two reasons. First, one of the main steps in Boltzmann’s argument was the partition of the phase space of a gas in regions of equal volume. Olivier Darrigol and Ulrich Hoyer have pointed out that, even if these volumes can be vanishingly small, they cannot really disappear, otherwise Boltzmann’s integrals are doomed to diverge.<sup>50</sup> By shifting the quantization from energy cells to regions of the phase space, Planck was therefore reinforcing the analogy between his procedure and Boltzmann’s. At the same time, the non-vanishing magnitude of the cell could be understood as an aftermath of the physical problem, an inconvenience of the incomplete analogy, not a flaw in the statistical formalism.

Second, both in December 1900 and in January 1901, Planck had stated that one fundamental assumption of his theory was the equiprobability of the complexions, but he had not clarified the status of this contention that, in his opinion, had to be decided empirically. As we will see more clearly in the next section, Boltzmann justified the equiprobability of his complexions by appealing to the Liouville theorem and a particular definition of probability. With his special partition of the phase space in 1906, Planck was able to introduce a justification of the equiprobability which relied on general electrodynamics and a universal constant only. He could validly feel that an important gap in his approach had been filled.

In the second edition of the *Vorlesungen* (1913), Planck further improves the position of the constant  $h$  in his theory by showing that it is closely related with a general thermodynamical result: Nernst’s theorem. The third law of thermodynamics discovered by Walther Nernst in 1905 entails the existence of an absolute definition of the entropy and, from Planck’s point of view, this implies an absolute definition of probability.<sup>51</sup> But probability hinges upon the partition of the phase space that, of course, must be also possible in an absolute way. Commenting the necessity of fixing a finite magnitude for the phase cell as a consequence of Nernst’s theorem, Planck says:

That such a definite finite quantity really exists is a characteristic feature of the theory we are developing, as contrasted with that due to Boltzmann, and forms the content of the so-called hypothesis of quanta. As readily seen, this

---

<sup>47</sup>(Planck, 1906, p. 153).

<sup>48</sup>(Planck, 1906, p. 156).

<sup>49</sup>The role played by the universal constants in Planck’s derivation has been stressed in (Badino & Robotti, 2001) and in (Gearhart, 2002).

<sup>50</sup>(Darrigol, 1988), (Hoyer, 1980).

<sup>51</sup>For an overview of the problems connected with Nernst’s theorem see (Kox, 2006).

is an immediate consequence of the proposition [...] that the entropy  $S$  has an absolute, not merely relative, value; for this, according to [ $S = k \log W$ ], necessitates also an absolute value for the magnitude of the thermodynamical probability  $W$ , which, in turn [...], is dependent on the number of complexions, and hence also on the number and size of the region elements which are used.<sup>52</sup>

Thus, by exploiting Nernst's thermodynamical result, that he had enthusiastically accepted from the outset, Planck is able to give to the finite magnitude of the cell in the phase space a meaning that is probabilistic and thermodynamic at the same time.

The previous discussion sheds some light on the relation between Planck's and Boltzmann's statistical formalism and on the more general issue of the internal consistency of Planck's theory. One of the main tenets of Kuhn's interpretation is that Planck developed a continuistic understanding of the combinatorial arguments in order to be consistent with the electromagnetic part of his theory that proceeded from the tradition of classical physics. However, Darrigol has pointed out that Planck's departures from Boltzmann's original procedure seem to imply that he was consistent with a part of the tradition he was appealing to and inconsistent with another part.<sup>53</sup> This selectivity in consistency looks rather arbitrary and difficult to justify. Martin Klein has proposed to characterize Planck's research program as "uniformly consistent," namely Planck was ready to tolerate some contradictions if only they allowed him to arrive at his final goal, a theoretical justification of the black-body radiation law.

However, I do not think that Planck's usage of the statistical formalism differs from Boltzmann's so remarkably or decisively as it was often assumed by the scholars. Or, at least, I do not think that Planck perceived a real fracture. The previous discussion has shown that Planck tried to apply Boltzmann's formalism through an analogy between a system of resonator and a system of molecules, but, since these two systems are physically different, he was forced to take account of the imperfections of the analogy. I would say that Planck was *analogically consistent* in his usage of Boltzmann's statistical doctrine: he was aware of the differences and that they mainly derived from the particular physical problem he was coping with. For instance, the counting procedure is a plain application of Boltzmann's idea of calculating the microstates consistent with a certain macrostate. What is different is the definition of a macrostate, because the spectral distribution Planck has to arrive at, is dissimilar from the velocity distribution of gas theory. In the former case, the distributions over the set of resonators are irrelevant, and they must be marginalized. Likewise, the maximization procedure was dispensable both because only the equilibrium has an empirical meaning for heat radiation and because of the particular concept of elementary disorder Planck had fostered. Lastly, Planck tried to embody the more marked difference—the finite magnitude of the energy element—in his statistical procedure through an interpretation of elementary region of the phase space and, eventually, through Nernst's theorem.

To be sure, the imperfections in the analogy also give rise to a number of ambiguities—especially of formal nature—that Planck exploited to keep an uncommitted position. As we have seen, it was statistically irrelevant, in his theory, if energy elements were distributed over resonators or resonators were distributed over energy cells. Similarly, he

---

<sup>52</sup>(Planck, 1913, p. 125).

<sup>53</sup>(Darrigol, 2001).



had the choice of using a maximization procedure or not. In his writings, Planck keeps shifting from one approach to the other without solving the dilemma: there is hardly more than some modest changes of emphasis. For instance, in the first edition of the *Vorlesungen*, Planck mentions the distribution of resonators over cells, but immediately thereafter he switches to the “faster and easier” original way. By contrast, in the second edition of the same book, published in 1913, Planck follows Boltzmann’s doctrine almost literally, introducing a distribution density function and maximizing it to find the equilibrium case. The original distribution of energy elements has only a marginal role. Once again, this change in emphasis is due to a modification of the physical perspective: in 1911, Planck had brought about his famous ‘second theory’ which relied on the quantum emission hypothesis and on the distribution of resonators over continuous energy cells, and the second edition of the *Vorlesungen* relies heavily on this new method. I will explain this point in the next section.

To sum up, it seems that the weak thesis is correct in suggesting that, as a matter of fact, Planck, for various reasons, adopted an uncommitted attitude towards most of the physical issues emerging from his combinatorial procedure, but the point is that Planck was also justified in doing so by the ambiguities and the differences that his analogical adaptation of Boltzmann’s statistics evoked. However, to complete the picture, we still need an answer to a fundamental question: why was Planck unwilling to draw physical inferences from his combinatorial procedure? This question concerns the main difference between Planck and Boltzmann and demands an analysis of their justifications of the introduction of statistics in physics. This analysis will add a further twist to our discussion.

## Organized Disorder

During his scientific life Boltzmann exposed his philosophical position in various essays and was involved in many scientific disputes especially concerning the necessity of the atomistic hypothesis and the so-called Energetic, but, unexpectedly enough, he rarely discusses the role of statistics in his theory. Some hints about his general opinion on this issue can be drawn from the final section of his 1868 paper.<sup>54</sup> In the first part of the paper, he undertakes the task of deriving Maxwell’s distribution by a classical analysis of the mechanical collisions and, in the second part, as we have seen above, he accomplishes the same goal employing a statistical argument. In the final section, Boltzmann justifies this two-pronged approach by indirectly explaining how statistical considerations enter his treatment of mechanical problems.<sup>55</sup>

However, his original argument is pretty obscure and I will try to reframe it in a more modern perspective. There are three ingredients:

- (1) Probability as sojourn time: the probability of a certain physical state represented by a region of the phase space of the system is the ratio between the time the

---

<sup>54</sup>(Boltzmann, 1868); see (Boltzmann, 1909, pp. I, 92–96). Another interesting point where Boltzmann displays his opinion on this topic is (Boltzmann, 1898, pp. 448–449).

<sup>55</sup>Of course, from a formal point of view, the main goal of the section is a proof of the uniqueness of Maxwell’s distribution by using the ergodic hypothesis (see for example (Uffink, 2007)), but I think that the particular view of the relation between statistics and mechanics implicit in this argument should not be underestimated.

system spends in that region and the total time considered (supposed to be very long).

- (2) Liouville's theorem: a well known result of general dynamics stating that if a system evolves according to the Hamiltonian equations of motion, then all the phase regions it passes through have the same volumes.
- (3) Ergodic hypothesis: a system will pass through all the phase regions consistent with its general constraints (e.g. the conservation of energy) provided that its evolution lasts long enough.

Boltzmann's argument goes as follows. Let us divide the trajectory time of the system into intervals of magnitude  $\Delta t$ , so that a phase trajectory for the system is a sequence of states:

$$\Sigma_t, \Sigma_{t+\Delta t}, \dots, \Sigma_{t+n\Delta t}.$$

From Liouville's theorem, it follows immediately that all these phase volumes are equal. But, since the system spends the same quantity of time  $\Delta t$  in each state, they are also equiprobable by definition (1). Therefore, the probability assigned to a certain state is proportional to the phase space volume of that state. If one now assumes that the ergodic hypothesis holds, then the system will pass through all the phase space regions consistent with its general conditions, and this means that, due to the deterministic evolution, there is only one trajectory filling up all the allowed phase space. Hence, one can describe the long run behaviour of the system by simply dividing the phase space into regions of equal volume (namely of equal probability) and calculating the number of regions corresponding to a certain macrostate. In other words, one can replace the temporal description of the long-run evolution of the system with a combinatorics on the phase space because all the space is filled up by a system trajectory.

Of course, this cannot be considered a formally satisfactory argument because of the problems connected to the ergodic hypothesis, but the general idea is clear enough: Boltzmann tries to introduce the usage of statistics in mechanics as an account of the behaviour of the mechanical system that is as rightful as the temporal description that the mechanics itself can provide, as long as some conditions hold on the system itself, notably the ergodic hypothesis. More importantly, the application of statistics does not rely on our ignorance of the detailed state of the system, namely on our epistemic status, but on a certain kind of behaviour of the mechanical system. The key point is that this justification amounts to an attempt of deeply *integrating* statistics and mechanics, of seeking for the mechanical conditions of an application of statistical arguments. He stresses this aspect also in the introduction of his 1872 paper:

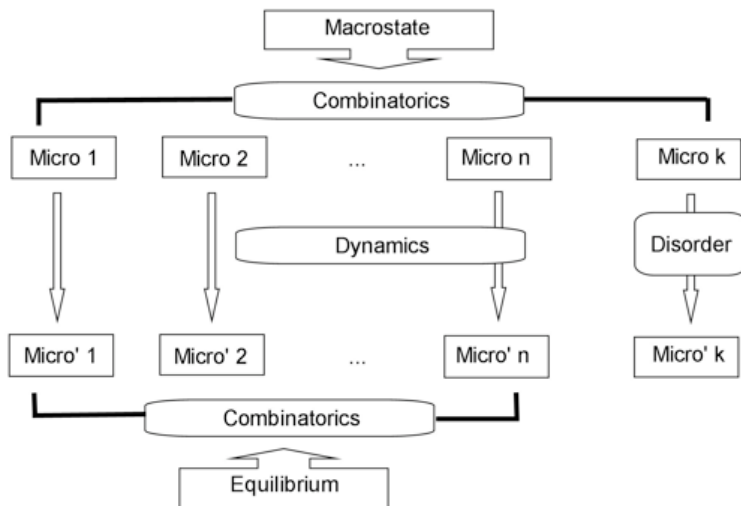
It would be an error to believe that there is an inherent indetermination in the theory of heat because of the usage of the laws of the calculus of probability. One should not mistake a law only incompletely proved, whose soundness is hence problematic, for a completely demonstrated law of the calculus of probability; the latter represents, like the result of any other calculus, a necessary consequence of given premises, and, if they are true, it is borne out in experience, as soon as many enough cases are observed what

is always the case in the theory of heat because of the enormous number of molecules.<sup>56</sup>

Planck's justification goes exactly in the opposite direction. The relation between statistics and electrodynamics is explained at the beginning of the fourth chapter of the first edition of the *Vorlesungen* and the starting point is the following dilemma:

Since with the introduction of probabilistic considerations into the electrodynamic theory of heat radiation, a completely new element, entirely unrelated to the fundamental principles of electrodynamics enters into the range of investigations, the question immediately arises, on the legitimacy and the necessity of such considerations. At first sight we might be inclined to think that in a purely electrodynamic theory there would be no room at all for probability calculations. Since, as everybody knows, the electrodynamic field equations together with the initial and boundary conditions determine uniquely the temporal evolution of an electrodynamic process, any consideration external to the field equations would be, in principle, unauthorized, and, in any case, dispensable. In fact, either they lead to the same results as the fundamental equations of electrodynamics and then they are superfluous, or they lead to different results and in this case they are wrong.<sup>57</sup>

However, Planck adds, the dilemma crops up from an incorrect understanding of the relation between the microlevel and the macrolevel. For the sake of convenience this relation can be summarized by another suitable scheme:



A certain macrostate is combinatorially related with many different microstates which evolve according to dynamical laws, in this case the laws of electrodynamics. However, Planck states, we cannot directly apply a dynamical analysis to the system because we do not know which of the many theoretically possible microstates actually holds. Our

<sup>56</sup>(Boltzmann, 1872); see (Boltzmann, 1909, pp. I, 317).

<sup>57</sup>(Planck, 1906, p. 129).

empirical measurements on the macrostate are able to supply only mean values, which are consistent with very many different combinations of exact values and then with many different microstates, consequently we do not have an unambiguous initial condition to start from. For this reason, the application of dynamical laws to the microstates is ambiguous.

Moreover, even if we actually know that the result of the dynamical evolution of the microstates is a set of new microstates whose overwhelming majority is combinatorially related to the equilibrium state, the plain application of combinatorial arguments is ambiguous as well, because there are some, very few indeed, microstates that might lead to an anti-thermodynamical evolution in which the entropy decreases. Thus, to replace the dynamical arguments with the combinatorial ones, and to retrieve an unambiguous (and deterministic, in Planck's view) picture, one has to hinder the anti-thermodynamical microstates. This result is achieved by the hypothesis of the elementary disorder which "states nothing more than that exceptional cases, corresponding to special conditions which exist between the separate quantities determining the state and which cannot be tested directly, do not occur in nature."

In the second edition, Planck verbalizes the difference between microstates and macrostates in an even more colorful way:

The microscopic state is the state as described by a mechanical or electro-dynamical observer; it contains the separate values of all coordinates, velocities, and field strengths. The microscopic processes, according to the laws of mechanics and electrodynamics, take place in a perfectly unambiguous way; for them entropy and the second principle of thermodynamics have no significance. The macroscopic state, however, is the state as observed by a thermodynamic observer; any macroscopic state contains a large number of microscopic ones, which it unites in a mean value. Macroscopic processes take place in an unambiguous way in the sense of the second principle, when, and only when, the hypothesis of the elementary disorder is satisfied.<sup>58</sup>

It is worthwhile noticing how deeply Planck's condition of disorder differ from Boltzmann's. Firstly there is a different relation to the statistical formalism: for Boltzmann, disorder is the prerequisite to introduce combinatorial arguments that can completely replace the dynamical ones because disorder permits all the theoretically allowed states, even the most improbable ones, to occur. By contrast, for Planck disorder is able to block the improbable states in order to pave the way to the triumph of the mean values. Secondly, while for Boltzmann disorder is a constitutive feature of the system, something that, in a sense, belongs to both the microlevel and the macrolevel (and allows the integration of both), for Planck it belongs exclusively to the microlevel, to a realm populated of hypothetical mechanical and electro-dynamical observers which see a completely different world utterly concealed to us. As it was already pointed out by Allan Needell and Olivier Darrigol, Planck's elementary disorder concerns the mysterious interaction of matter and radiation and hence it is part of the uncontrollable and inaccessible microworld.

Therefore, the statistical arguments are not another, equally rightful, viewpoint of looking at mechanical problems, but the only way at our disposal of figuring out what

---

<sup>58</sup>(Planck, 1913, p. 121).

is going on in the complicated and unreachable realm of the constituents of matter and radiation. Consequently, Planck merely considers the statistical arguments as a conceptual device to represent a chaotic situation and to perform useful calculations, but he does not deem them as a basis for understanding the physical world. This point clearly emerges in the second edition of the *Vorlesungen*. The general architecture of the book is remarkably dissimilar from the first edition. In particular, while in the first edition the statistical arguments were a means to overcome the issues left open by the dynamical approach, in the second edition the dynamical part of the theory is constrained to satisfy the general results obtained from the statistical analysis because “the only type of dynamical law admissible is one that will give for the stationary state of the oscillators exactly the distribution densities [...] calculated previously.”<sup>59</sup>

The new dynamical law is the famous quantum emission hypothesis that Planck introduces with the following words:

... we shall assume that the emission does not take place continuously, as does the absorption, but that it occurs only at certain definite times, suddenly, in pulse, and in particular we assume that an oscillator can emit energy only at the moment when its energy of vibration,  $U$ , is an integral multiple  $n$  of the quantum of energy  $\epsilon = h\nu$ . Whether it then really emits or whether its energy of vibration increases further by absorption will be regarded as a matter of chance. This will not be regarded as implying that there is no causality for emission; but the processes which cause the emission will be assumed to be of such a concealed nature that for the present their laws cannot be obtained by any but statistical methods.<sup>60</sup>

Even though the statistical part takes the leading role in the second edition of the *Vorlesungen*, the dynamical assumptions it provides are not to be meant as realistic ones. In fact, statistical considerations remain nothing but a convenient mean to paraphrase a hidden reality.

## Who Cares for the Microworld?

The discussion in the previous sections seems to suggest that we should be very cautious in attributing any commitment to Planck on the grounds of his usage of the statistical formalism. Admittedly, Planck tried to follow Boltzmann’s formalism as faithfully as possible and the deviations are to be ascribed to the imperfections of the analogy, i.e. to the differences in the physical problems, but his attitude towards the statistical arguments was quite the opposite of Boltzmann’s. The Austrian physicist had tried to integrate mechanics and statistics by showing that the conditions for applying statistical argument are to be sought in some particular mechanical behaviour. On the contrary, Planck is quite clear in confining the statistical arguments into the impenetrable processes taking place at the microlevel: in Planck’s view, electromagnetism and statistics are completely dis-integrated. This general attitude and the formal ambiguities of the statistical procedures formed the ground for his contention that there were no conclusions to be drawn from the combinatorial fact that discrete energy elements were distributed

---

<sup>59</sup>(Planck, 1913, p. 152).

<sup>60</sup>(Planck, 1913, p. 153).

over resonators or, alternatively, that resonators were distributed over continuous energy cells. In this concluding section, I would like to discuss in more detail the concept of virtual observer, the disorder and the resulting relation between the dis-integration of electrodynamics and statistics and the construction of the microworld.

Boltzmann's microworld is assembled by conceptual elements coming from the macro-world, e.g. molecules as mechanical points or centers of force, elastic collisions and so on, and it is also characterized by the emergence of the statistical formalism as a mean of investigating physical reality. By integrating the statistical formalism with the mechanical one, typical of the macrolevel, Boltzmann establishes a new direction for the conceptual flow that eventually leads him to reinterpret the macroscopic laws in terms of the statistical viewpoint. The statistical interpretation of the second law is the most remarkable result of this bi-directional conceptual interaction between micro- and macroworld. The conceptual interaction between micro- and macroworld is bi-directional because Boltzmann integrates the formal ways of describing them and, in particular, integrates statistics with the rest of physical knowledge. On the contrary, by dis-integrating dynamical and statistical formalism and by reducing the latter to a computational device, Planck ends up with a microworld that is completely shaped by the macroscopic conceptual structure and it is unable to support any reinterpretation of the macrophenomena. In fact, what makes up Planck's microworld is only conceived as a way of representing, by means of macroscopic concepts, the mysterious and unobservable business of the interaction between matter and radiation. Furthermore, since statistics is completely separated from the rest of the physical knowledge, the statistical formalism has little to say both on the macroworld and on the microworld: statistics is not supposed to give us a description of how the world is, it is only supposed to give us a way of handling chaotic situations.

The particular relation between macro- and microworld is clearly presented in the Columbia lectures of 1909. As we have seen, in the second edition of the *Vorlesungen*, Planck uses the concept of "virtual" (micro- or macro-) observer, to figure out a more intuitive definition of the micro- and macrostate. Actually, this concept had made its first appearance in the third lecture of the series mentioned above as an important element of his general argument for the justification of the usage of statistics.

Again, Planck points out that the contradiction between the reversibility of the microphenomena and the irreversibility of the thermodynamical laws stems from different definitions of state. The physical state envisioned by a micro-observer, that is "a physicist [...] whose senses are so sharpened that he is able to recognize each individual atom and to follow it in its motion,"<sup>61</sup> is fundamentally different from the state of a usual macro-observer, because the former observes exact values and the latter only means. However, since the virtual micro-observer is nothing but a projection of a macroscopic one, Planck is shaping the issue of the contradictory relation between micro- and macroworld in terms of the macroworld itself. Thus, it is not surprising that the answer as well embodies the primacy of the macrolevel as can be verified by further comparing Boltzmann's and Planck's notion of disorder.

For Boltzmann the elementary disorder is a feature concerning the individual configurations of molecules and, more importantly, is the ultimate justification of the introduction of statistical arguments and the final warrant of their equivalence with the

---

<sup>61</sup>(Planck, 1915, p. 47).

mechanical ones. In his *Gastheorie*, Boltzmann distinguishes the concepts of molar and molecular disorder. The former concerns the fact that the mean values of the mechanical quantities, e.g. the molecular velocity, do not vary from a spatial region to another occupied by the gas. The latter is, significantly enough, introduced by means of its opposite, the molecular order:

If the arrangement of the molecules also exhibits no regularities that vary from one finite region to another—if it is thus molar-disordered—then nevertheless groups of two or a small number of molecules can exhibit definite regularities. A distribution that exhibits regularities of this kind can be called molecular-ordered. We have a molecular-ordered distribution if—to select only two example from the infinite manifold of possible cases—each molecule is moving towards its nearest neighbor, or again if each molecule whose velocity lies between certain limits has ten much slower molecules as nearest neighbors.<sup>62</sup>

While Boltzmann's concept of disorder directly dives into the details of the molecular arrangements, and realizes the possibility of a statistical interpretation of thermodynamics, Planck's analogous notion only deals with the coherence of the Fourier components of radiation (a macroscopic concept) and, even more remarkably, it is supposed to block any anti-thermodynamical evolution. The difference is extremely important and scarcely stressed in the secondary literature. If a system is molecular-ordered in Boltzmann's sense, then only a subset of the theoretically possible states will actually be realized, whereas, if the system is molecular-disordered, there is nothing, in the initial configuration, that prevents all possible states from occurring and this is precisely the condition for applying statistical methods. In other words, Boltzmann's disorder does not block a particular kind of evolution, but simply rules out the occurring of 'conspiratory' configurations where only a subset of evolutions is possible.<sup>63</sup>

By contrast, Planck conceives the elementary disorder as a limitation on the statistical formalism itself because some of the theoretically possible configurations cannot take place. As a result, one obtains a new definition of microstate:

The micro-observer needs only to assimilate in his theory the physical hypothesis that all those special cases in which special exceptional conditions exist among the neighboring configurations of interacting atoms do not occur in nature, or, in other words, that the micro-states are in elementary disorder. Then the uniqueness of the macroscopic process is assured and with it, also, the fulfillment of the principle of increase of entropy in all direction.<sup>64</sup>

Planck's change of meaning and function of the elementary disorder has far-reaching consequences.<sup>65</sup> By means of the virtual micro-observer and of the elementary disorder, Planck foists upon the constitution and the formalism of the microworld a series of

---

<sup>62</sup>(Boltzmann, 1898, p. 40).

<sup>63</sup>Cf. for example (Boltzmann, 1898, p. 451): "only singular states that *continually* deviate from probable states must be excluded" (italics added).

<sup>64</sup>(Planck, 1915, p. 50).

<sup>65</sup>A further support of the thesis that Planck's notion of elementary disorder differs from Boltzmann's comes again from the third lecture. In a note, he claims that Poincare's recurrence theorem calls for a careful formulation of the hypothesis of the elementary disorder in order to avoid the, even only

constraints coming from the macroworld. Since Planck's parasitic microworld is completely shaped by means of conceptual material and formal requirement relying on the macro-level, and since its characteristic formalism is conceived to be nothing but a set of computational devices, the only conceptual feedback it can warrant are those leading to derivations of the macro-laws, like the black-body radiation law.<sup>66</sup>

Analogously, Planck's conversion to Boltzmann's point of view seems to concern rather the notion of irreversibility as an 'emerging' phenomenon than the statistical interpretation of the macroworld:

[I]rreversibility does not depend upon an elementary property of a physical process, but rather depends upon the ensemble of numerous disordered elementary processes of the same kind, each one of which individually is completely reversible, and upon the introduction of the macroscopic method of treatment.<sup>67</sup>

Of course, the emerging notion of irreversibility is only the premise of Boltzmann's conception, but Planck is not in the position of accepting the consequence. Ultimately, his way of justifying the usage of statistics in physics is a justification of his ambiguous—or prudent—use of the statistical formalism as well.

Thus, we arrive at a similar conclusion to the weak thesis we have discussed above, but on a different ground. Actually, Planck was not interested in committing himself on the issue of continuity (also) because he did not need to. By breaking the Boltzmannian conceptual links between statistics and dynamics, between micro- and macrolevel that would have forced him to take a clear position, by constructing a microworld completely shaped by the macroworld, and by denying an autonomous status to the statistical formalism, he could peacefully stay away from dangerous connections between apparently incompatible formalisms.

Our analysis provides a possible explanation why Planck could maintain the reticent position he actually maintained about the quantum in his published writings. But, at the same time, it also provides an unexpected new argument for the continuity view. The monodirectionality of the conceptual exchange by which Planck builds up his microworld suggests that he was unwilling to ascribe to the microphenomena any feature that we do not observe at the macrolevel. Of course, he was not explicit on this point and this cannot be called a clear commitment, because it concerns the relation between micro- and macroworld from a broad methodological viewpoint. Therefore, a slightly different position emerges, a position one can name a 'weak version of the continuity thesis:' Planck did not manifest any commitment on the reality of the quantum and, as

---

theoretical, possibility of a low-entropy evolution. In particular, Planck's way out is the statement that "absolutely smooth walls do not exist in nature" (Planck, 1915, p. 51). On the contrary Boltzmann reckoned the recurrence theorem in its original formulation perfectly consistent with his notion of disorder: "[t]he fact that a closed system of a finite number of molecules [...] finally after an inconceivably long time must again return to the ordered state, is therefore not a refutation, but rather indeed a confirmation of our theory" ((Boltzmann, 1898, p. 443)).

<sup>66</sup>Incidentally, the monodirectionality of this relation between micro- and macroworld is part of the reason why Planck, even acknowledging the generality of Boltzmann's approach, did not develop a statistical mechanics. Instead a decisive move in this direction was performed by Einstein who restored the bidirectional conception of micro- and macroworld and the autonomy of the statistical formalism. See for example (Renn, 1997) and (Uffink, 2005).

<sup>67</sup>(Planck, 1915, p. 97).



a matter of fact, exploited all the ambiguities of his statistical formalism to associate his theory as little as possible to any clear statement on this issue, but this strategy demands a separation between statistics and dynamics, micro- and macroworld, and Planck's choice for the macroworld suggests that his preference went to a view of energy as a continuous quantity.

The thrust of this argument is that even if Planck had adopted the same statistical arguments as Boltzmann, he understood the role of statistics in a completely different way and, more importantly, he was unwilling to integrate the statistical considerations with the physical knowledge his theory relied on. Thus, though Planck's and Boltzmann's name are often associated in the history of quantum theory, they seem to be an "odd couple," because, like the characters of the famous movie, their attitudes on the fundamental problems could not have been more diverging.

This perspective also gives us some clues to understand the relations between Planck and his contemporaries. In fact, Planck's attitude was not a completely idiosyncratic one. On the contrary, he was placing himself within an illustrious thermodynamic tradition including Clausius and Helmholtz. According to this tradition, the hypotheses concerning the uncontrollable microlevel have to be avoided as long as they are not absolutely necessary and, if this is the case, only minimally and cautiously introduced. Famously, Clausius, who was Planck's guiding spirit in thermodynamics, refused to use the distribution function until his late years and when he was forced to bring up some statistical assumptions on the behaviour of the constituents he always limited himself to what was strictly necessary to arrive at his final result. Helmholtz, Planck's predecessor in Berlin, endorsed a pure thermodynamics even when mechanical concepts were used, like in his papers on the monocycle.<sup>68</sup>

On the other side of the river stood Boltzmann, who was not afraid of introducing bold assumptions on the behaviour of the molecules and of coping with them using the conceptual tools of statistics. Paul Ehrenfest as well as Albert Einstein belonged to the same tradition and, not unsurprisingly, they did not understand and sharply criticized Planck's usage of statistical arguments. Einstein, for instance, showed his legacy to Boltzmann's train of thought in his light quantum paper where he derives the existence of energy elements of free radiation from their statistical behaviour. That was exactly the kind of inference Planck could not consent. This fundamental fracture affected a large part of the relations between statistical mechanics and the early quantum theory.

## References

- Bach, A. (1990). Boltzmann's Probability Distribution of 1877. *Archive for History of Exact Sciences*, 41, 1–40.
- Badino, M., & Robotti, N. (2001). Max Planck and the constants of Nature. *Annals of Science*, 58, 137–162.
- Boltzmann, L. (1868). Studien über das Gleichgewicht der lebendigen Kraft zwischen bewegten materiellen Punkten. *Wiener Berichte*, 58, 517–560.

---

<sup>68</sup>On this 'Berlin's style' in physics see (Jurkowitz, 2002).

- Boltzmann, L. (1872). Weitere Studien über das Wärmegleichgewicht unter Gasmolekülen. *Wiener Berichte*, 66, 275–370.
- Boltzmann, L. (1877). Über die Beziehung zwischen dem zweiten Hauptsatze der mechanischen Wärmetheorie und der Wahrscheinlichkeitsrechnung respektive den Sätzen über das Wärmegleichgewicht. *Wiener Berichte*, 76, 373–435.
- Boltzmann, L. (1898). *Vorlesungen über Gastheorie* (S. G. Brush, Trans.). Leipzig: Barth.
- Boltzmann, L. (1909). *Wissenschaftliche Abhandlungen*. Leipzig: Barth.
- Büttner, J., Renn, J., & Schemmel, M. (2003). Exploring the Limits of Classical Physics: Planck, Einstein, and the Structure of a Scientific Revolution. *Studies in History and Philosophy of Modern Physics*, 34, 37–59.
- Costantini, D., & Garibaldi, U. (1997). A Probabilistic Foundation of Elementary Particle Statistics. Part I. *Studies in History and Philosophy of Modern Physics*, 28 (4), 483–506.
- Costantini, D., Garibaldi, U., & Penco, M. A. (1996). Ludwig Boltzmann alla nascita della meccanica statistica. *Statistica*, 3, 279–300.
- Darrigol, O. (1988). Statistics and Combinatorics in Early Quantum Theory. *Historical Studies in the Physical Science*, 19, 18–80.
- Darrigol, O. (1991). Statistics and Combinatorics in Early Quantum Theory, II: Early Symptoma of Indistinguishability and Holism. *Historical Studies in the Physical Science*, 21, 237–298.
- Darrigol, O. (2000). Continuities and discontinuities in Planck's Akt der Verzweiflung. *Annalen der Physik*, 9, 851–860.
- Darrigol, O. (2001). The Historians' Disagreements over the Meaning of Planck's Quantum. *Centaurus*, 43 (3–4), 219–239.
- Ehrenfest, P., & Kamerlingh Onnes, H. (1915). Vereinfachte Ableitung der kombinatorischen Formel, welche der Planckschen Strahlungstheorie zugrunde liegt. *Annalen der Physik*, 46, 1021–1024.
- Einstein, A. (1924). Quantentheorie des einatomigen idealen Gases I. *Berliner Berichte*, 261–267.
- Galison, P. (1981). Kuhn and the Quantum Controversy. *The British Journal for the Philosophy of Science*, 32 (1), 71–85.
- Garber, E. (1976). Some reactions to Planck's Law, 1900–1914. *Studies in History and Philosophy of Science*, 7 (2), 89–126.
- Gearhart, C. A. (2002). Planck, the Quantum, and the Historians. *Physics in Perspective*, 4, 170–215.

- Heilbron, J. (1986). *The Dilemmas of an Upright Man. Max Planck as Spokesman for German Science*. Berkeley: University of California Press.
- Hoyer, U. (1980). Von Boltzmann zu Planck. *Archive for History of Exact Sciences*, 23, 47–86.
- Jost, R. (1995). Planck-Kritik des T. Kuhn. In *Das Märchen vom Elfenbeinernen Turm. Reden und Aufsätze*. Berlin: Springer.
- Jurkowitz, E. (2002). Helmholtz and the liberal unification of science. *Historical Studies in the Physical and Biological Sciences*, 32 (2), 291–317.
- Kangro, H. (1970). *Vorgeschichte des Planckschen Strahlungsgesetzes*. Wiesbaden: Steiner.
- Klein, M. J. (1962). Max Planck and the Beginnings of the Quantum Theory. *Archive for History of Exact Sciences*, 1, 459–479.
- Klein, M. J. (1963a). Einstein's First Papers on Quanta. *Natural Philosopher*, 2, 59–86.
- Klein, M. J. (1963b). Planck, Entropy, and Quanta, 1901–1906. *Natural Philosopher*, 1, 83–108.
- Klein, M. J. (1964). Einstein and the Wave-Particle Duality. *Natural Philosopher*, 3, 3–49.
- Klein, M. J. (1966). Thermodynamics and Quanta in Planck's Work. *Physics Today*, 19 (11), 23–32.
- Klein, M. J., Shimony, A., & Pinch, T. J. (1979). Paradigm Lost? A Review Symposium. *Isis*, 70, 429–440.
- Koch, M. (1991). From Boltzmann to Planck: On continuity in scientific revolutions. In W. R. Woodward & R. S. Cohen (Eds.), *World Views and Scientific Discipline Formation* (pp. 141–150). Amsterdam: Kluwer Academic.
- Kox, A. J. (2006). Confusion and clarification: Albert Einstein and Walther Nernst's heat theorem, 1911–1916. *Studies in History and Philosophy of Modern Physics*, 37, 101–114.
- Kuhn, T. (1978). *Black-Body Theory and the Quantum Discontinuity, 1894–1912*. Oxford: Oxford University Press.
- Kuhn, T. (1984). Revisiting Planck. *Historical Studies in the Physical Science*, 14(2), 232–252.
- Natanson, L. (1911). Über die statistische Theorie der Strahlung. *Physikalische Zeitschrift*, 12, 659–666.
- Needell, A. (1980). *Irreversibility and the Failure of Classical Dynamics: Max Planck's Work on the Quantum Theory, 1900–1915*. Unpublished PhD Dissertation, University of Michigan, Ann Arbor.

- Planck, M. (1900a). Entropie und Temperatur strahlender Wärme. *Annalen der Physik*, 4 (1), 719–737.
- Planck, M. (1900b). Zur Theorie des Gesetzes der Energieverteilung im Normalspektrum. *Verhandlungen der Deutschen Physikalische Gesellschaft*, 2, 237–245.
- Planck, M. (1901). Über das Gesetz der Energieverteilung im Normalspektrum. *Annalen der Physik*, 4 (4), 553–563.
- Planck, M. (1906). *Vorlesungen über die Theorie der Wärmestrahlung*. Leipzig: Barth.
- Planck, M. (1913). *The Theory of Heat Radiation* (M. Masius, Trans.). New York: Dover.
- Planck, M. (1915). *Eight Lectures on Theoretical Physics* (A. P. Wills, Trans.). New York: Dover.
- Planck, M. (1958). *Physikalische Abhandlungen und Vorträge*. Braunschweig: Vieweg & Sohn.
- Planck, M. (1972). *Planck's Original Papers in Quantum Physics* (D. t. Haar & S. G. Brush, Trans.). London: Taylor&Francis.
- Renn, J. (1997). Einstein's Controversy with Drude and the Origin of Statistical Mechanics. *Archive for History of Exact Sciences*, 51 (4), 315–354.
- Rosenfeld, L. (1936). La premiere phase de l'evolution de la theorie des quanta. *Osiris*, 2, 148–196.
- Uffink, J. (2005). Insuperable difficulties: Einstein's statistical road to molecular physics. *Studies in History and Philosophy of Modern Physics*, 37, 36–70.
- Uffink, J. (2007). Compendium of the foundations of classical statistical mechanics. In J. Butterfield & J. Earman (Eds.), *Philosophy of Physics* (pp. 923–1074). Amsterdam: North Holland.



# 3 Poincaré's Electromagnetic Quantum Mechanics

ENRICO R. A. GIANNETTO

*The rise of quantum physics is considered by outlining the historical context in which different conceptions of Nature (mechanistic, thermodynamic and electromagnetic ones) were in competition to give a foundation to physics. In particular, the roots of quantum physics within the electromagnetic conception of Nature and Poincaré's quantum electromagnetic mechanics are analysed.*

## Introduction

### Conceptions of Nature

As well known, in the late XIXth century physics was no more mechanics only, but also thermodynamics and electrodynamics. This new situation implied the problem of the very foundations of physics, and the correlated issue of the hierarchical relations among these different physical disciplines.<sup>1</sup> There were at least four different “fighting” conceptions of Nature. The so-called *Energetic* conception of Nature, which was looking at energy as the fundamental unifying concept of physics and had its most important proponents in Georg Helm (1851–1923) and Wilhelm Ostwald (1853–1932).

The *Thermodynamic* conception of Nature, which had energy, entropy and system as fundamental concepts and was looking at thermodynamics as the real foundation block of physics. Its major exponents were Pierre Duhem (1861–1916) and Max Planck (1858–1947).

The *Mechanical* conception of Nature, which was the most conservative one as searching for a mechanical reduction of the other physical disciplines and of all the physical concepts in terms of mass, space and time by means of the models of material point and action at-a-distance forces. Hermann von Helmholtz (1821–1894), Heinrich Hertz (1857–1894) and Ludwig Boltzmann (1844–1906) were the most representative scientists of this perspective.

The *Electromagnetic* conception of Nature, based on the concepts of field, energy and charge was looking at electromagnetism theory as the foundation level of the other physical disciplines. Among the physicists who gave the most relevant contributions to this perspective there are: Hendrik Antoon Lorentz (1853–1928), Joseph Larmor (1857–1942), Wilhelm Wien (1864–1928), Max Abraham (1875–1922) and Henry Poincaré (1854–1912). The electromagnetic conception of Nature has deep roots in the history of

---

<sup>1</sup>R. McCormach, C. Jungnickel, *Intellectual Mastery of Nature: Theoretical Physics from Ohm to Einstein*, I–II, The University of Chicago Press, Chicago 1986, II vol., pp. 211–253; E. Giannetto, *Saggi di storie del pensiero scientifico*, Sestante for Bergamo University Press, Bergamo 2005, pp. 299–321.

mankind and certainly has been developed by the elaboration of the Brunian-Leibnizian physics and tradition. On one side, it has been developed within the German physics or *Naturphilosophie*, on the other side mainly within English physics.

William Gilbert (1540–1603) and then the same Johannes Kepler (1571–1630) were thinking about magnetism as the force which rules the order of our cosmos, of our Copernican world, and Athanasius Kircher (1602–1680) developed a theology of magnetism and of the magnetic Divine Universal Love.

Indeed, after the process by which Newtonian gravitation was reduced from a divine active force to a passive property of inertial matter and Newton's theology of gravitation was given up and mechanistic conception of Nature came to dominate, electricity came back to be considered the way to a new vitalistic conception of Nature. Electricity was considered an active force which could have been the origin of animated life, that is an active vital force, the Leibniz' internal *vis viva*, as well as the same *psyché* within things—a sort of electric unconscious—or the same Anima Mundi. Many theologians and physicists, like Prokop Divisch (1698–1765), Friedrich Christoph Oetinger (1702–1782), Johan Ludwig Fricker (1729–1766), Gottlieb Friedrich Rösler (1740–1790), developed a very theology and psychology of electricity. The controversy on animal electricity at the end of XVIII and at the beginning of XIX century between Luigi Galvani (1737–1798) and Alessandro Volta (1745–1827), gave another turn to the consideration of the problem and its resolution with the dominance Volta's perspective and his presentation, in 1800, of the first 'electric machine', the battery, pointed out the victory of the mechanistic view and the reduction of life to mechanisms to which even electricity could have been assimilated. It was the romantic physicist Johan Wilhelm Ritter (1776–1810) who turned Volta's interpretation upside down, stating that, because there was not a specific animal electricity, the whole Nature was a living and animated being just for the presence of electricity. Electric fluid was the *psyché* of everything. Romanticism continued to develop these ideas and Franz Anton Mesmer (1734–1815) spoke about animal magnetism, about a magnetic fluid as a universal soul, about *psyché* as a magnetic nervous fluid, about psychical sickness as magnetic diseases which could be healed by magnetic hypnotism.

Maxwell electromagnetism had shown that physical reality was not only inertial and passive matter, but also dynamical, active electromagnetic field, irreducible to a mechanical matter model. Furthermore, Maxwell equations present vacuum solutions, that is in absence of charged matter: electromagnetic field exists even when there is no matter. Thus, the possibility of a new non-dualistic view of physical reality was considered: if matter cannot exist without electromagnetic field and electromagnetic field can exist without matter, electromagnetic field could be the only physical reality and matter could be derived from the field.

### Electromagnetic Conception of Nature and Relativity

Usually, the electromagnetic conception of Nature has been considered as superseded by the developments of XXth century physics. However, a deep historical inquiry shows that the electromagnetic conception of Nature is at the roots of both the relativistic and quantum transformations of physics.

Concerning relativity, the 1900, 1902, 1904 and (5 June) 1905 papers written by

Poincaré<sup>2</sup> show as special relativity dynamics derived from, and was a first realization of, the electromagnetic conception of nature. Einstein's (30 June) 1905 paper was only an incomplete mechanistic version of this new dynamics. This historical recognition is also fundamental to understand the first reception of special relativistic dynamics in all countries, and in particular in Italy.

A first complete presentation of this new dynamics appeared in the July 1905 paper written by Poincaré and published in 1906.<sup>3</sup> In this paper the new dynamics was presented as an invariant one by the Lorentz-Poincaré transformation group, and it was derived by Maxwell's theory of electromagnetism and contained also a theory of gravitation (absent in Einstein's 1905 paper).

The starting point was electromagnetic self-induction phenomenon related to the so-called radiation reaction. When a charged particle is submitted to the action of an electromagnetic field, it is accelerated and it irradiates. This radiation modifies the field and the new field modifies the acceleration of the particle, which again irradiates and so on. In this way, the electromagnetic field depends on all the time derivatives of position up to the infinite one. This means that there is also a contribution to the field force proportional to the acceleration, the coefficient of which involves an electromagnetic mass, that is an electromagnetic contribution to the particle inertia.

At this point, the question was: is it possible that mechanical (inertial and gravitational) mass was not a primitive concept and indeed is wholly due to this electromagnetic effect? Poincaré, among other scientists, realized that this was the case also for non-charged matter as long as is constituted by charged particles: that is mechanical mass was nothing else than electromagnetic mass, and electromagnetic mass is not a static fixed quantity but depends on velocity. Mass is so related to the electromagnetic field energy by the today well-known (now considered from a mechanistic and not electromagnetic perspective) equation:  $m = E_{e.m.field}/c^2$ .

If mass is nothing else than electromagnetic field energy and charge can be defined, via Gauss' theorem, to the electric field flux through a certain space surface, matter can be completely understood in terms of the electromagnetic field, and it has also active and dynamical features beyond the passive and inertial ones. If mass must be understood in terms of the electromagnetic field, mechanics must be derived by electromagnetism theory which becomes the fundamental theory of physics. If mass changes with velocity, Newtonian mechanics is no more valid and must be modified. The new mechanics must have the same invariance group of electromagnetic theory, that is the Lorentz-Poincaré transformation group, to which a new relativity principle and a new gravitation theory (even gravitational mass changes with velocity) must also be conformed.

From Poincaré's perspective even gravitation is of electromagnetic origin. However, the new gravitational theory developed by Einstein's general relativity theory did not take count of this idea.<sup>4</sup> David Hilbert, simultaneously with Einstein, developed the

---

<sup>2</sup>H. Poincaré, *La mesure de temps*, in *Revue de Métaphysique et Morale* **6**, 1 (1898); H. Poincaré, *La théorie de Lorentz et le principe de réaction*, *Arch. Néerl.* **5**, 252 (1900); H. Poincaré, *La Science et l'Hypothèse*, Flammarion, Paris 1902; H. Poincaré, *L'état actuel et l'avenir de la Physique mathématique*, in *Bulletin des Sciences Mathématiques* **28**, 302 (1904); H. Poincaré, *Sur la dynamique de l'électron*, in *Comptes Rendus de l'Académie des Sciences* **140**, 1504 (1905).

<sup>3</sup>H. Poincaré, *Sur la dynamique de l'électron*, in *Rendiconti del Circolo Matematico di Palermo* **21**, 129 (1906).

<sup>4</sup>A. Einstein, *Die Feldgleichungen der Gravitation*, in *Königlich Preußische Akademie der Wissenschaften*



same gravitational field equations.<sup>5</sup>

The problem of the priority of Einstein or Hilbert, even if historically important, is not the relevant point. Indeed, the fundamental point is that in Hilbert's perspective matter ( $T_{\mu\nu}$ ) is considered as of electromagnetic origin: Hilbert and Einstein equations are mathematically equivalent, but they do not have the same physical meaning. Hilbert's point of view is related to a synthesis of the electromagnetic theory of Gustav Mie (1868–1957)<sup>6</sup> and Einstein theory of gravitation: Hilbert equations give automatically also Maxwell generalized electromagnetic field equations, which follow from the space-time structure induced by “electromagnetic matter.”<sup>7</sup>

Thus, it can be traced an evolution line, within the electromagnetic conception of Nature, which started from Poincaré's special-relativistic dynamics and through Mie's theory lead to Hilbert's general-relativistic dynamics. And indeed, by the Hilbert electromagnetic general relativity, that is by the Hilbert electromagnetic theory of matter and gravitation, the cosmic and universal order came back to be related to magnetism as in the first proposals by Gilbert, Kepler and Kircher.

## Electromagnetic Conception of Nature and Quantum Physics

The rising of quantum physics is conventionally related to the works of Planck during the years 1899–1900.<sup>8</sup> However, Joseph Larmor, within an electromagnetic conception of Nature, was working to understand the atomic structure of matter in terms of the electromagnetic field at least since 1893.<sup>9</sup> After leaving the idea of a “vortex atom”, he considered the electrons as vortices into the sea of the electromagnetic field: this idea lead him to what, many years later, was called a “quantum atom”. Electrons as rotations into the electromagnetic field constitute stable, stationary non-radiant configurations of atoms: these configurations correspond to given discrete values of the conserved angular momentum. Radiation is emitted or absorbed by atoms by impulses only when these

---

(Berlin), *Sitzungsberichte*, 1915, pp. 844–847.

<sup>5</sup>D. Hilbert, *Die Grundlagen der Physik (Erste Mitteilung)*, in *Nachrichten von der Königlich Gesellschaft der Wissenschaften zu Göttingen, Mathematisch-physikalische Klasse*, Berlin 1916, pp. 395–407.

<sup>6</sup>G. Mie, *Grundlagen einer Theorie der Materie, Erste Mitteilung*, in *Annalen der Physik* **37** (1912) pp. 511–534; *Zweite Mitteilung*, in *Annalen der Physik* **39** (1912) pp. 1–40; *Dritte Mitteilung*, in *Annalen der Physik* **40** (1913) pp. 1–66.

<sup>7</sup>E. R. A. Giannetto, *Einstein, Hilbert and the Origins of the General Relativity Theory*, in press.

<sup>8</sup>M. Jammer, *The Conceptual Development of Quantum Mechanics*, McGraw-Hill, New York 1966, pp. 1–61; M. Planck, *Über irreversible Strahlungsvorgänge*, in *Berliner Berichte*, 18 May 1899, 440 (1899); M. Planck, *Zur Theorie des Gesetzes der Energieverteilung im Normalspektrum*, in *Verhandlungen der Deutschen Pysikalischen Gesellschaft* **2** (14 December), 237 (1900), engl. tr., *On the Theory of the Energy Distribution Law of the Normal Spectrum*, in D. ter Haar, *The Old Quantum Theory*, Pergamon Press, Oxford 1967, pp. 82–90.

<sup>9</sup>J. Larmor, *A Dynamical Theory of the Electric and Luminiferous Medium*, abstract, in *Proc. Roy. Soc.* **54**, 438 (1893); part I, in *Phil. Trans. Roy. Soc.* **185**, 719 (1894); part II abstract, in *Proc. Roy. Soc.* **58**, 222 (1895); part II, in *Phil. Trans. Roy. Soc.* **186**, 695 (1895); part III abstract, in *Proc. Roy. Soc.* **61**, 272 (1897); part III, in *Phil. Trans. Roy. Soc.* **A190**, 205 (1897); J. Larmor, *On the theory of the magnetic influence on spectra; and on the radiation of moving ions*, in *Phil. Mag. (5)* **44**, 503 (1897); J. Larmor, *Aether and Matter*, Cambridge University Press, Cambridge 1900; B. Giusti Doran, *Origins and Consolidation of Field Theory in Nineteenth-Century Britain: From the Mechanical to the Electromagnetic View of Nature*, in *Historical Studies in the Physical Sciences* **6**, (1975), Princeton University Press, Princeton.

configurations change in respect to the minimal total energy. Thus, emission of radiation and loss of energy were not related to the absolute translations of the electron as an accelerated, charged material particle, but to the relative changes (within the atoms) of the inertial rotational motions constituting electrons (in any stable state the change of velocity in a period is zero). This idea furnished an explanation of atomic spectra and even a prediction of the Zeeman effect. This electromagnetic conception of the atomic matter structure, that is the recognition of these atomic matter structures within the electromagnetic field, Larmor understood, would be also the key to the calculus of specific heats in terms of internal energy and equal partition of energy within the kinetic theory of gases.

Planck wanted to show the universality of thermodynamics and its second principle showing that it holds also for electromagnetic phenomena. Planck was forced to use Boltzmann's statistical thermodynamics concept of entropy, but showed that thermodynamics cannot be reduced to mechanics because heat is not only disordered matter motion but also electromagnetic radiation and that thermodynamics could be deduced by electromagnetism theory too. In 1900 Planck introduced discrete values of energy as heuristic tool within statistical thermodynamics of radiation to fit black-body radiation distribution experimental data. That is, energy was treated by Planck not as a continuous mathematical variable, but discrete:

$$E = nh\nu$$

where  $n$  is an integral number and so energy is given by an integral multiple of the product of a universal constant  $h = 6.5510^{-27}$  erg/sec with the physical dimension of an action and the radiation frequency. Planck's words made reference to "energy elements" (*Energieelemente*), but Planck did not want to introduce an essential discontinuity within Nature but only to solve by the mathematical artifact of discreteness the problem to fit experimental data: he did not want to modify classical physics or to make a revolution. In 1899 Planck had already introduced this constant naming it "b" and not "h", it did not denote an action and it was a constant in the different theoretical context of finding an absolute system of natural units of measure.

The first actual physical meaning to this constant was given not by Einstein, but by Larmor in 1902 within his electromagnetic conception of Nature.<sup>10</sup> Following Larmor, Planck's constant was not related to a mathematical artifact but had to be interpreted in terms of the relationship between matter and (ether) electromagnetic field, that is as the ratio between matter energy (given by electromagnetic field energy) and radiation frequency. Planck's constant, for Larmor, was a quantum of the conserved angular momentum to be related to atomic electrons considered as vortices within electromagnetic field.

Larmor proposed also to leave the abstract oscillator model of matter used by Planck and to take count of the actual electromagnetic nature and origin of matter. This implied

---

<sup>10</sup>J. Larmor, *Theory of Radiation*, in *Encyclopedia Britannica* 8 (vol. XXXII of the complete work), 120 (1902), Black, London. J. Larmor, *On the application of the method of entropy to radiant energy*, in *Reports Brit. Assoc. Adv. Sci. 1902*, 546 (1903) (abstract of a paper presented at the Belfast meeting); J. Larmor, *On the statistical and thermodynamical relations of radiant energy*, in *Proc. Roy. Soc. (London)* A83, 82 (1909); J. Larmor, *Preface* (1911) to *The Scientific Papers of S. B. McLaren*, Cambridge University Press, Cambridge 1925.

to use the simple idea of ‘elementary receptacles of energy’, that is of cells in the phase space of physical systems. This idea was deduced from the consideration of the nature of radiation, constituted by discrete elements given by short trains of simple undulations. The phase space reformulation of Planck’s problem lead to the discreteness of the atomic conserved angular momentum from which was deduced the discreteness of energy. J. W. Nicholson in 1912<sup>11</sup> explored this explanation of the atomic structure and his work was the starting point of Niels Bohr’s model.

From Larmor’s perspective, from the electromagnetic conception of Nature, the discrete, discontinuous, quantum nature of matter and radiation is easily understood because matter is derived from the fundamental physical reality given by the electromagnetic field. Thus, electromagnetic field must present wave but also corpuscular aspects to explain the origin of matter, and matter particles must present corpuscular but also wave aspects as long as they derive from the electromagnetic field.

Bohr<sup>12</sup> reconsidered Nicholson’s model but completely changing its meaning: atom was no more understood in terms of the electromagnetic conception of Nature but in terms of an axiomatic approach in which the meaning of Planck’s constant is no more given by the electromagnetic nature of the atomic matter structure but by an abstract quantum of mechanical action. Bohr followed Arnold Sommerfeld’s perspective<sup>13</sup> which presumed to understand all the things in terms of an a priori assumed and unexplained constant, that is Planck’s constant: electromagnetic as well as thermodynamic and mechanical models were considered to be no more suitable because electromagnetic field theory as well as thermodynamics and mechanics must be reformulated in order to fit experiments and to overcome the problem of their incompatibility. However, Sommerfeld and Bohr seem to not understand that their interpretation of Planck’s constant was mechanical and this put mechanics at the fundamental level of physics, restating a new mechanistic perspective. It happened something like to the procedure of axiomatization which lead to the loss of electromagnetic meaning to the light velocity constant  $c$  in the mechanistic version of relativity dynamics given by Einstein. The meaning variance of a revolutionary item ( $c$  as well as  $h$ ), together with the change in its “title” (“Universal Constant”), is a well known process which leads to a restoration, to a dogma to be understood “mechanically” and to a myth of the foundations of a new religion as well as a new scientific theory.

From Larmor’s perspective, Planck’s statistical thermodynamics of electromagnetism implied that classical electromagnetism continuous variables lose meaning and cannot be precisely determined, but only probabilistically just in order to derive matter corpuscles from the electromagnetic field.

In 1905–1906 Einstein<sup>14</sup>, as well as he had done with Poincaré’s new electromagnetic relativistic dynamics, by criticizing Planck noted the discontinuous and probabilistic character of radiation but inverted Larmor’s perspective and introduced the quanta of light to reduce electromagnetism (as a statistical theory) to corpuscular mechanics.

---

<sup>11</sup>J. W. Nicholson, in *Monthly Notices of the Royal Astronomical Society* **72**, 49, 139, 677, 693, 729 (1912).

<sup>12</sup>N. Bohr, in *Philosophical Magazine* **26**, 1, 476, 857 (1913).

<sup>13</sup>A. Sommerfeld, in *Physikalische Zeitschrift* **12**, 1057 (1911).

<sup>14</sup>A. Einstein, *Über einen die Erzeugung und Verwandlung des Lichtes betreffenden heuristischen Gesichtspunkt*, in *Annalen der Physik* **17**, 132 (1905); A. Einstein, *Zur Theorie der Lichterzeugung und Lichtabsorption*, in *Annalen der Physik* **20**, 199 (1906).

## Poincaré's New Quantum Electromagnetic Mechanics

In 1911 there was the famous first Solvay Conference on the problems raised by Planck's hypothesis and Einstein's quanta. Poincaré was present and participated actively to the debate: here, he understood immediately that physics was at the threshold of the deepest revolution ever happened. It could imply the renounce to the differential equations as (means to formulate) physical laws.<sup>15</sup> In 1911–1912, Poincaré wrote and published two important papers:<sup>16</sup> the first was presented to the *Académie des Sciences* on 4 December 1911. Poincaré showed that Planck's black body law implies necessarily the quanta hypothesis and these new discontinuous characters of light and electromagnetic field cannot be understood in terms of the old corpuscular mechanics, and, on the contrary, these changes within electromagnetic theory imply a new mechanics. Indeed, if mechanics has to be built on electromagnetism and electromagnetism must be changed, then also mechanics must be modified: there must be a new “electromagnetic dynamics”.

Poincaré proceeded in this way:<sup>17</sup> let be a system, whose state is defined by  $n$  parameters  $x_1, x_2, x_3, \dots, x_n$ . Let be the evolution laws of these parameters formulated by the following differential equations:  $\frac{dx_k}{dt} = u_k$ .

Let be  $WdJ$  the probability that the point representing the system state be in the volume  $dJ$  of the  $x_k$ -space; then  $W$ , the probability density, must satisfy the equation

$$\sum_k \partial \left( \frac{W u_k}{\partial x_k} \right) = 0,$$

where the  $u_k$  are the generalized velocities and the equation, as it will be shown, is the same continuity equation that must be satisfied by the Jacobi last multiplier  $K$ .<sup>18</sup>

When we deal with classical mechanics indeed we can write the Jacobi equations of

<sup>15</sup>See the *Discussion du rapport de M. Einstein*, in M. P. Langevin et M. de Broglie (eds.), *La théorie du rayonnement et les quanta. Rapports et discussions de la Réunion tenue à Bruxelles, du 30 Octobre au 3 Novembre 1911 sous les auspices de M. E. Solvay*, Gauthier-Villars, Paris 1912, pp. 436–454, in particular p. 451 and *Abhandlungen der deutschen Bunsengesellschaft* **7**, pp. 330–364;

<sup>16</sup>H. Poincaré, *Sur la théorie des quanta*, in *Comptes Rendus de l'Académie des Sciences*, v. **153** (1912), pp. 1103–1108, reprinted in H. Poincaré, *Œuvres de Henri Poincaré*, I–XI, Gauthier-Villars, Paris 1934–1956, v. **IX**, pp. 620–625; *Sur la théorie des quanta*, in *Journal de Physique théorique et appliquée*, v. **2** (1912), pp. 5–34, reprinted in *Œuvres*, v. **IX**, op. cit., pp. 626–653; *L'hypothèse des quanta*, in *Revue Scientifique*, v. **50** (1912), pp. 225–232, reprinted in *Œuvres*, v. **IX**, op. cit., pp. 654–668 and as chapter 6 in H. Poincaré, *Dernières pensées*, Flammarion, Paris 1913; H. Poincaré, *Les rapports de la matière et l'éther*, in *Journal de physique théorique et appliquée*, ser 5, **2** (1912), pp. 347–360, reprinted in *Œuvres*, v. **IX**, op. cit., pp. 669–682 and as chapter 7 in H. Poincaré, *Dernières pensées*, op. cit.. See also: H. Poincaré, *L'évolution des lois*, conference delivered at the Congresso di Filosofia di Bologna on 8 April 1911, in *Scientia*, v. **IX** (1911), pp. 275–292, reprinted as chapter 1 in *Dernières pensées*, op. cit.

<sup>17</sup>See footnote 16.

<sup>18</sup>C. G. J. Jacobi, in *Crelle's Journal* **XXVII** (1844) p. 199 and **XXIX** p. 213, 388; A. R. Forsyth, *A Treatise on Differential Equations*, MacMillan, London 1885, sixth edition 1948, pp. 356–366; E. Whittaker, *A Treatise on the Analytical Dynamics of Particles and Rigid Bodies*, Cambridge University Press, Cambridge 1904, fourth edition 1960, pp. 267–287; R. H. Fowler, *Statistical Mechanics—The Theory of the Properties of Matter in Equilibrium*, Cambridge University Press, Cambridge 1929, second edition 1936, reprinted in 1955, pp. 11–15; D. Buoccaletti, G. Pucacco, *Theory of Orbits, vol. I, Integrable Systems and Non-perturbative Methods*, Springer Verlag, Berlin 1996, pp. 61–72.

motion in the canonical form:

$$\frac{dq_i}{dt} = \frac{\partial T}{\partial p_i} \quad \text{and} \quad \frac{dp_i}{dt} = -\frac{\partial T}{\partial q_i} + Q_i$$

where

$$Q_i = \sum_k (X_k \frac{\partial x_k}{\partial q_i} + Y_k \frac{\partial y_k}{\partial q_i} + Z_k \frac{\partial z_k}{\partial q_i})$$

are generalized forces.

These equations are more general than Hamilton's ones, because they do not presuppose the existence of a potential function.

The Jacobi last multiplier is so defined:

$$0 = \frac{d(\log K)}{dt} + \sum_k \partial \left( \frac{\partial T}{\partial p_k} \right) + \sum_k \partial \left( \frac{\partial p_k}{\partial dt} \right)$$

From this equation it follows:

$$\frac{1}{K} \frac{dK}{dt} + \sum_k \partial \left( \frac{dq_k}{dt} \right) + \sum_k \partial \left( \frac{-\frac{\partial T}{\partial q_k} + Q_k}{\partial p_k} \right) = 0$$

For  $K$  different from zero, it yields:

$$\frac{dK}{dt} + K \sum_k \partial \left( \frac{dq_k}{dt} \right) + \sum_k \partial \left( \frac{-\frac{\partial T}{\partial q_k} + Q_k}{\partial p_k} \right) = 0$$

and so in the other coordinates:

$$\frac{dK}{dt} + K \sum_k \frac{\partial u_k}{\partial x_k} = 0$$

Then, it can be written:

$$\frac{dK}{dt} + K \operatorname{div} \vec{u} = 0$$

and so:

$$\frac{\partial K}{\partial t} + (\operatorname{div} K) \vec{u} + K \operatorname{div} \vec{u} = 0$$

And finally the following continuity equation is obtained:

$$\frac{\partial K}{\partial t} + \operatorname{div}(K \vec{u}) = 0$$

If Hamilton's equations

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \quad \text{and} \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}$$

hold, then  $\frac{\partial Q_k}{\partial p_k} = 0$  and

$$\frac{dq_i}{dt} = \frac{\partial T}{\partial p_i} \quad \text{and} \quad \frac{dp_i}{dt} = -\frac{\partial T}{\partial q_i}$$

Thus, it can be deduced that:

$$\sum_k \partial \frac{u_k}{\partial x_k} = \sum_k \partial \left( \frac{\partial T}{\partial p_k} \right) - \sum_k \partial \left( \frac{\partial T}{\partial q_k} \right) = 0$$

If  $\text{div}(K\vec{u}) = 0$ , that is the current is stationary, then

$$(\text{div } K)\vec{u} + K \text{ div } \vec{u} = 0$$

and so from

$$\text{div } \vec{u} = 0$$

it follows

$$(\text{div } K)\vec{u} = 0$$

Therefore, for  $K$  different from  $K = K(t)$ , that is for  $K$  independent from time, it yields:

$$\frac{dK}{dt} = \text{div}(K\vec{u}) = 0,$$

and so

$$\frac{dK}{dt} = K \text{ div } \vec{u} + (\text{div } K)\vec{u} = 0,$$

and finally

$$\frac{dK}{dt} = (\text{div } K)\vec{u} = 0,$$

so that  $K$  is independent even from the  $x_k$ , that is  $K$  is a constant.

Thus, we can choice  $K = 1$  and then it is obtained

$$\text{div}(K\vec{u}) = K \text{ div } \vec{u} = 0$$

and so

$$\text{div } \vec{u} = 0$$

with Hamilton's equations satisfied. Otherwise, if  $K$  is not constant and in general it depends from  $t$  and from the  $x_k$ , it is

$$\sum_k \partial \left( \frac{K u_k}{\partial x_k} \right) = 0$$

that is the same equation that holds for the probability density  $W$ , and so  $W = K$ : probability density is the Jacobi last multiplier. The condition  $W = K = 1$ , as Dugas has remarked<sup>19</sup>, corresponds to the complete homogeneity of the possibility that the system state representative point is everywhere in the phase space of the  $q_k$  and the  $p_k$ .

---

<sup>19</sup>R. Dugas, *Histoire de la mécanique*, Griffon, Neuchâtel 1955, English tr. by J. R. Maddox, *A History of Mechanics*, Dover, New York 1988, pp. 552–553 and 622–626. For other comments to Poincaré's papers, see: M. Planck, *Henri Poincaré und die Quantentheorie*, in *Acta Mathematica* 1, **38** (1921) pp. 387–397; H. A. Lorentz, *Deux Mémoires de Henri Poincaré sur la Physique mathématique*, in H. Poincaré, *Oeuvres de Henri Poincaré*, op. cit., **11**, pp. 247–261; P. Langevin, *L'oeuvre d'Henri Poincaré. Le physicien*, in *Revue de Métaphysique et de morale*, Supplément au n. 5 (1913), pp. 675–718; R. McCormach, *Henri Poincaré and the quantum theory*, in *Isis* **58** (1967), pp. 37–55.

Thus, Poincaré proposed to introduce a new Jacobi last multiplier, that is a new probability density in phase space, different from unity and given by an essential discontinuous function just to obtain Planck's law and not Rayleigh-Jeans equation of equipartition.

$W$  must be a function containing factors  $w = w(e_k)$  which are zero for values of energy  $e_k$  different from a multiple of the quantum  $e$ . This property is introduced to give a finite energy electromagnetic radiation: thus, mechanics must be modified to take count of electromagnetic variables, that is of the modified electrodynamics which Planck's law requires. This can be realized trivially by assuming that all the mechanical forces, and so all the forms of exchange of energy, are of electromagnetic nature. The new mechanics is a new quantum electromagnetic mechanics.

This new quantum electromagnetic mechanics, as Poincaré conceived it, is a theory for an isolated system, and rigorously only for the whole universe: the evolution dynamics of the universe thus results to be discontinuous and the universe would jump discontinuously from a state to another one. This implies that it is not possible to distinguish a continuous range of intermediate states and instants too in which no change is present in the universe, and so it yields a discontinuous time: atoms of time must be introduced. This was the first time a *quantum time* was introduced.

If  $W$  is an essentially discontinuous function all the equations involving it must be modified by replacing integrals with sums and derivatives and differentials with finite variations, which correspond to quantum discontinuous jumps.

Thus, it yields a finite variation equation for  $W$ :

$$\sum_k \frac{\Delta(W(\frac{\Delta x_k}{\Delta t}))}{\Delta x_k} = 0$$

This is an equation for a discontinuous quantum "density matrix" in the phase space or in the action-angle space. The discontinuity of the  $W$  function corresponds to the impossibility of simultaneously determining the separate probability distributions of coordinates and momenta as continuous variables, in such a way that a minimum size for phase space cell exists and it is given by

$$\Delta q \Delta p = h$$

This is the finite difference relation which must replace the integral equation for an elementary phase space cell introduced by Planck and quoted by Poincaré: this relation implies the mutual dependent variability of coordinates and momenta, which furthermore must vary in jumps.

Poincaré's new equations of motion are the first form of new quantum mechanical equations and can be compared to the successive most general form of quantum mechanical Liouville equations for density matrix<sup>20</sup> when it is impossible to define a Schrödinger wave function: however, Poincaré's equations represent a more radical shift from classical mechanics, because are finite variation equations. From Poincaré perspective, continuity cannot be saved even writing an equation for the probability density, because this must be an essentially discontinuous function. Poincaré's equations are more general than

---

<sup>20</sup>P. Carruthers and M. M. Nieto, *Phase and Angle Variables in Quantum mechanics*, in *Reviews of Modern Physics* **40** (1968) p. 411.

Schrödinger's ones in a further respect: they do not presuppose the possibility to define a potential function for the interaction, because are derived from Jacobi equations.

Dugas<sup>21</sup> has shown (even by neglecting the potential problem) that in Schrödinger's quantum mechanics the Jacobi last multiplier is given by  $\psi^*\psi$  defined in configuration space and in Dirac's spinorial quantum relativistic mechanics by  $\psi_k^*\psi_k$  as continuous functions. However, following Poincaré, even probability density functions are discontinuous and physical laws can no more be represented by differential equations.

From this perspective, electromagnetism cannot be reduced to mechanics, but, on the contrary, mechanics must be modified again and in more radical way than by the relativistic electromagnetic dynamics: mechanics must be intrinsically probabilistic even for only one material particle, because the origin of matter is electromagnetic and electromagnetic radiation is discontinuous.

Poincaré's new electromagnetic discontinuous mechanics based on a discontinuous electromagnetic action was mathematically very difficult for the other physicists (Jacobi last multiplier technique was used in celestial mechanics) and was not understood at all: thus, this first form of a new revolutionary electromagnetic quantum mechanics was not accepted.

## Concluding Remarks

Only after many years, in 1925, Heisenberg<sup>22</sup> stated the necessity of, and posed the basis for, a new quantum mechanics: his starting point was not the electromagnetic conception of Nature, but an operational perspective. Heisenberg showed that at the atomic or microphysical level the only measurable variables were the electromagnetic variables of frequency and intensity of electromagnetic radiation absorbed or emitted by electrons within atoms. From this point of view, mechanical variables, as long as they are not directly measurable and cannot be objects of absolute experimentation, intuition or visualization at the atomic microphysical level, must be redefined in terms of such measurable electromagnetic variables. This implied, as then stated in 1927 by Heisenberg himself<sup>23</sup>, a fundamental indeterminacy of mechanical variables. If physical reality is only what can be experimentally measured, from Heisenberg's perspective the electromagnetic conception of Nature can be deduced without any aprioristic assumption. Its deduction follows merely from the request of an operational definition of physical variables at the microscopic level.

Unfortunately, this original derivation and foundation of quantum mechanics has been completely forgotten and removed. It was for ideological reasons that mechanics must be maintained independent from electromagnetism and at the foundation level of the physical sciences. This priority of mechanics is related to the mechanistic conception of Nature. Considering Nature and the other non-human living beings as machines, that is as inert and passive matter, is the pre-condition to avoid any ethical problem in respect

---

<sup>21</sup>See footnote 19

<sup>22</sup>W. Heisenberg, *Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen*, in *Zeitschrift für Physik* **33**, 879 (1925); M. Born, W. Heisenberg and P. Jordan, *Zur Quantenmechanik II*, in *Zeitschrift für Physik* **35**, 557 (1926).

<sup>23</sup>W. Heisenberg, *Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik*, in *Zeitschrift für Physik* **43**, 172 (1927).



of Nature and the other non-human living beings and to the complete violent dominion over, and exploitation of, Nature and the other living beings.

## References

1. R. McCormach, C. Jungnickel, *Intellectual Mastery of Nature: Theoretical Physics from Ohm to Einstein*, I–II, The University of Chicago Press, Chicago 1986, II vol., pp. 211–253; E. Giannetto, *Saggi di storie del pensiero scientifico*, Sestante for Bergamo University Press, Bergamo 2005, pp. 299–321.
2. H. Poincaré, *La mesure de temps*, in *Revue de Métaphysique et Morale* **6**, 1 (1898); H. Poincaré, *La théorie de Lorentz et le principe de réaction*, *Arch. Néerl.* **5**, 252 (1900); H. Poincaré, *La Science et l'Hypothèse*, Flammarion, Paris 1902; H. Poincaré, *L'état actuel et l'avenir de la Physique mathématique*, in *Bulletin des Sciences Mathématiques* **28**, 302 (1904); H. Poincaré, *Sur la dynamique de l'électron*, in *Comptes Rendus de l'Académie des Sciences* **140**, 1504 (1905).
3. H. Poincaré, *Sur la dynamique de l'électron*, in *Rendiconti del Circolo Matematico di Palermo* **21**, 129 (1906).
4. A. Einstein, *Die Feldgleichungen der Gravitation*, in *Königlich Preußische Akademie der Wissenschaften (Berlin), Sitzungsberichte*, 1915, pp. 844–847.
5. D. Hilbert, *Die Grundlagen der Physik (Erste Mitteilung)*, in *Nachrichten von der Königlich Gesellschaft der Wissenschaften zu Göttingen, Mathematisch-physikalische Klasse*, Berlin 1916, pp. 395–407.
6. G. Mie, *Grundlagen einer Theorie der Materie, Erste Mitteilung*, in *Annalen der Physik* **37** (1912) pp. 511–534; *Zweite Mitteilung*, in *Annalen der Physik* **39** (1912) pp. 1–40; *Dritte Mitteilung*, in *Annalen der Physik* **40** (1913) pp. 1–66.
7. E. R. A. Giannetto, *Einstein, Hilbert and the Origins of the General Relativity Theory*, in press.
8. M. Jammer, *The Conceptual Development of Quantum Mechanics*, McGraw-Hill, New York 1966, pp. 1–61; M. Planck, *Über irreversible Strahlungsvorgänge*, *Berliner Berichte*, 18 May 1899, 440 (1899); M. Planck, *Zur Theorie des Gesetzes der Energieverteilung im Normalspektrum*, in *Verhandlungen der Deutschen Pysikalischen Gesellschaft* **2** (14 December), 237 (1900), engl. tr., *On the Theory of the Energy Distribution Law of the Normal Spectrum*, in D. ter Haar, *The Old Quantum Theory*, Pergamon Press, Oxford 1967, pp. 82–90.
9. J. Larmor, *A Dynamical Theory of the Electric and Luminiferous Medium*, abstract, in *Proc. Roy. Soc.* **54**, 438 (1893); part I, in *Phil. Trans. Roy. Soc.* **185**, 719 (1894); part II abstract, in *Proc. Roy. Soc.* **58**, 222 (1895); part II, in *Phil. Trans. Roy. Soc.* **186**, 695 (1895); part III abstract, in *Proc. Roy. Soc.* **61**, 272 (1897); part III, in *Phil. Trans. Roy. Soc.* **A190**, 205 (1897); J. Larmor, *On the theory of the magnetic influence on spectra; and on the radiation of moving ions*,

- in *Phil. Mag. (5)* **44**, 503 (1897); J. Larmor, *Aether and Matter*, Cambridge University Press, Cambridge 1900; B. Giusti Doran, *Origins and Consolidation of Field Theory in Nineteenth-Century Britain: From the Mechanical to the Electromagnetic View of Nature*, in *Historical Studies in the Physical Sciences* **6**, (1975), Princeton University Press, Princeton.
10. J. Larmor, *Theory of Radiation*, in *Encyclopedia Britannica* **8** (vol. XXXII of the complete work), 120 (1902), Black, London. J. Larmor, *On the application of the method of entropy to radiant energy*, in *Reports Brit. Assoc. Adv. Sci. 1902*, 546 (1903) (abstract of a paper presented at the Belfast meeting); J. Larmor, *On the statistical and thermodynamical relations of radiant energy*, in *Proc. Roy. Soc. (London)* **A83**, 82 (1909); J. Larmor, *Preface* (1911) to *The Scientific Papers of S. B. McLaren*, Cambridge University Press, Cambridge 1925.
  11. J. W. Nicholson, in *Monthly Notices of the Royal Astronomical Society* **72**, 49, 139, 677, 693, 729 (1912).
  12. N. Bohr, in *Philosophical Magazine* **26**, 1, 476, 857 (1913).
  13. A. Sommerfeld, in *Physikalische Zeitschrift* **12**, 1057 (1911).
  14. A. Einstein, *Über einen die Erzeugung und Verwandlung des Lichtes betreffenden heuristischen Gesichtspunkt*, in *Annalen der Physik* **17**, 132 (1905); A. Einstein, *Zur Theorie der Lichterzeugung und Lichtabsorption*, in *Annalen der Physik* **20**, 199 (1906).
  15. See the *Discussion du rapport de M. Einstein*, in M. P. Langevin et M. de Broglie (eds.), *La théorie du rayonnement et les quanta. Rapports et discussions de la Réunion tenue à Bruxelles, du 30 Octobre au 3 Novembre 1911 sous les auspices de M. E. Solway*, Gauthier-Villars, Paris 1912, pp. 436–454, in particular p. 451 and *Abhandlungen der deutschen Bunsengesellschaft* **7**, pp. 330–364;
  16. H. Poincaré, *Sur la théorie des quanta*, in *Comptes Rendus de l'Académie des Sciences*, v. **153** (1912), pp. 1103–1108, reprinted in H. Poincaré, *Œuvres de Henri Poincaré*, I–XI, Gauthier-Villars, Paris 1934–1956, v. **IX**, pp. 620–625; *Sur la théorie des quanta*, in *Journal de Physique théorique et appliquée*, v. **2** (1912), pp. 5–34, reprinted in *Œuvres*, v. **IX**, op. cit., pp. 626–653; *L'hypothèse des quanta*, in *Revue Scientifique*, v. **50** (1912), pp. 225–232, reprinted in *Œuvres*, v. **IX**, op. cit., pp. 654–668 and as chapter 6 in H. Poincaré, *Dernières pensées*, Flammarion, Paris 1913; H. Poincaré, *Les rapports de la matière et l'éther*, in *Journal de physique théorique et appliquée*, ser 5, **2** (1912), pp. 347–360, reprinted in *Œuvres*, v. **IX**, op. cit., pp. 669–682 and as chapter 7 in H. Poincaré, *Dernières pensées*, op. cit. See also: H. Poincaré, *L'évolution des lois*, conference delivered at the Congresso di Filosofia di Bologna on 8 April 1911, in *Scientia*, v. **IX** (1911), pp. 275–292, reprinted as chapter 1 in *Dernières pensées*, op. cit..
  17. C. G. J. Jacobi, in *Crelle's Journal* **XXVII** (1844) p. 199 and **XXIX** p. 213, 388; A. R. Forsyth, *A Treatise on Differential Equations*, MacMillan, London 1885, sixth edition 1948, pp. 356–366; E. Whittaker, *A Treatise on the Analytical*

*Dynamics of Particles and Rigid Bodies*, Cambridge University Press, Cambridge 1904, fourth edition 1960, pp. 267–287; R. H. Fowler, *Statistical Mechanics—The Theory of the Properties of Matter in Equilibrium*, Cambridge University Press, Cambridge 1929, second edition 1936, reprinted in 1955, pp. 11–15; D. Buoccaletti, G. Pucacco, *Theory of Orbits, vol. I, Integrable Systems and Non-perturbative Methods*, Springer Verlag, Berlin 1996, pp. 61–72.

18. R. Dugas, *Histoire de la mécanique*, Griffon, Neuchâtel 1955, English tr. by J. R. Maddox, *A History of Mechanics*, Dover, New York 1988, pp. 552–553 and 622–626. For other comments to Poincaré’s papers, see: M. Planck, *Henri Poincaré und die Quantentheorie*, in *Acta Mathematica* 1, **38** (1921) pp. 387–397; H. A. Lorentz, *Deux Mémoires de Henri Poincaré sur la Physique mathématique*, in H. Poincaré, *Oeuvres de Henri Poincaré*, op. cit., **11**, pp. 247–261; P. Langevin, *L’oeuvre d’Henri Poincaré. Le physicien*, in *Revue de Métaphysique et de morale*, Supplément au n. 5 (1913), pp. 675–718; R. McCormach, *Henri Poincaré and the quantum theory*, in *Isis* **58** (1967), pp. 37–55.
19. P. Carruthers and M. M. Nieto, *Phase and Angle Variables in Quantum mechanics*, in *Reviews of Modern Physics* **40** (1968) p. 411.
20. W. Heisenberg, *Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen*, in *Zeitschrift für Physik* **33**, 879 (1925); M. Born, W. Heisenberg and P. Jordan, *Zur Quantenmechanik II*, in *Zeitschrift für Physik* **35**, 557 (1926).
21. W. Heisenberg, *Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik*, in *Zeitschrift für Physik* **43**, 172 (1927).

# 4 Einstein's Miraculous Argument of 1905: The Thermodynamic Grounding of Light Quanta

JOHN D. NORTON

*A major part of Einstein's 1905 light quantum paper is devoted to arguing that high frequency heat radiation bears the characteristic signature of a microscopic energy distribution of independent, spatially localized components. The content of his light quantum proposal was precarious in that it contradicted the great achievement of nineteenth century physics, the wave theory of light and its accommodation in electrodynamics. However the methods used to arrive at it were both secure and familiar to Einstein in 1905. A mainstay of Einstein's research in statistical physics, extending to his earliest publications of 1901 and 1902, had been the inferring of the microscopic constitution of systems from their macroscopic properties. In his statistical work of 1905, Einstein dealt with several thermal systems consisting of many, independent, spatially localized components. They were the dilute sugar solutions of his doctoral dissertation and suspended particles of his Brownian motion paper.<sup>1</sup>*

## 4.1 Introduction

The year 1905 is now commonly known as Einstein's "year of miracles." In it, in a series of extraordinary papers, the 26-year-old clerk in the Bern patent office redirected the course of physics. Those five papers were, in order of their dates of submission and publication:

- Light quantum ("photoelectric effect") paper (Einstein, 1905a). Einstein inferred from the thermal properties of high frequency heat radiation that it behaves thermodynamically as if constituted of spatially localized, independent quanta of energy.
- Einstein's doctoral dissertation (Einstein, 1905b). Einstein used known physical properties of sugar solutions (viscosity, diffusion) to determine the size of sugar molecules.

---

<sup>1</sup>I am grateful to participants of the conference HQ-1: Conference on the History of Quantum Physics (July 2–6, 2007, Max Planck Institute for the History of Science) for helpful discussion after presentation of this paper. The present paper is based on Norton (2006). For an informal version, see also "Atoms Entropy Quanta: Einstein's Statistical Physics of 1905" under Goodies on [www.pitt.edu/~jdnorton](http://www.pitt.edu/~jdnorton) I also thank Continental Airlines for Flight CO 0097 from Berlin to Newark, July 7, 2007, on which portions of this text were written.

- Brownian motion paper (Einstein, 1905c). Einstein predicted that the thermal energy of small particles would manifest as a jiggling motion, visible under the microscope and providing the most direct support then available for the molecular-kinetic approach to thermal systems.
- Brownian motion paper (Einstein, 1905c). Einstein predicted that the thermal energy of small particles would manifest as a jiggling motion, visible under the microscope and providing the most direct support then available for the molecular-kinetic approach to thermal systems.
- Special relativity (Einstein, 1905d). Einstein urged that maintaining the principle of relativity in electrodynamics requires a new theory of space and time.
- $E = mc^2$  (Einstein, 1905e). Einstein showed that changing the energy  $E$  of a body changes its inertia  $m$  in accord with  $E = mc^2$ .

In a letter of May 2005, Einstein described the first four of these papers to his friend Conrad Habicht. It is striking and noteworthy that Einstein singles out the first paper, the light quantum paper, for an extraordinary description “The [first] paper deals with radiation and the energy properties of light and is very revolutionary,...” (*Papers*, Vol. 5, Doc. 27)

It is not hard to see why Einstein would single out his light quantum paper in this way—and that remains true if we include consideration of the later  $E = mc^2$  paper, which had not been conceived at the time of Einstein’s May letter. All but the light quantum paper develop or complete programs of research of nineteenth century physics, sometimes in quite inspired ways. The two statistical papers, the dissertation and the Brownian motion paper, advance decisively a program of research in thermal systems developed by Maxwell, Boltzmann and others in the nineteenth century, the molecular kinetic theory of heat. The special relativity paper establishes the real significance of the Lorentz covariance of Maxwell’s electrodynamics, that it betokened a new theory of space and time. Finally, the  $E = mc^2$  paper took a result from electrodynamics, that light energy has momentum, and used the principle of relativity to extend it to all forms of energy.

The light quantum paper was different. The signal achievements of nineteenth century physics were: the wave theory of light and the recognition that Newton’s authoritative corpuscular theory fails; Maxwell’s electrodynamics and its development and perfection by Hertz, Lorentz and others; and the synthesis of the two in the single luminous idea that light waves just are electromagnetic waves. Einstein’s light quantum paper threatened this great synthesis in its fundamentals. Light, Einstein now asserted, did not always behave as a wave. Sometimes it behaved as if its energy was localized into independent points in space. Indeed with this idea of the light quantum, Einstein initiated a reappraisal of the physical constitution of light that is not entirely resolved over a hundred years later.

My concern in this paper is to answer the question of how even an Einstein could have the courage to propose this revolutionary notion of the light quantum. My analysis will depend on distinguishing the *content* of the light quantum hypothesis from the *methods* Einstein used to arrive at it. The content of Einstein’s discovery was quite unanticipated: it asserted that high frequency light energy exists in independent, spatially localized

points. However the *method* of Einstein's discovery was familiar and secure. His research program in statistical physics from his first publication of 1901 returned repeatedly to the question: How can we infer the microscopic properties of matter from its macroscopic properties? For example, the dissertation and Brownian motion paper of 1905 were devoted to analyzing dilute sugar solutions and very small particles suspended in a fluid. That is, they were devoted to studying thermal systems whose statistical constitution was similar to the one Einstein attributed to high frequency light energy, in that they consist of many, independent, spatially localized, points (sugar molecules, small particles). As a result Einstein was adept at dealing with such systems and, most importantly, quite sensitive to how such systems appear macroscopically.

My goal here is not to give a fine-grained reconstruction of Einstein's pathway to the light quantum. Many pathways are compatible with the analysis I shall give. My goal is to show that, if we locate Einstein's light quantum paper against the background of electrodynamic theory, its claims are so far beyond bold as to be foolhardy. However, if we locate Einstein's light quantum paper against the background of his work in statistical physics, its methods are an inspired variation of ones repeatedly used and proven effective in other contexts on very similar problems.

The miraculous argument and its similarity to Einstein's other projects from that time will be outlined in Section 4.2 and 4.3. In Section 4.4, I will note that the ideal gas law is a more familiar signature of the microscopic constitution Einstein inferred for radiation; and in Section 4.5 I will explain why I believe Einstein did not use it in his argument. Finally, in Section 4.6, I will review a remarkably simple and much repeated argument that Einstein advanced in his light quantum paper for what he named Boltzmann's principle: " $S = k \log W$ ." I will argue that the maddening imprecision of the argument was needed because it was to be applied to systems of light quanta whose full properties were correspondingly imprecisely known.

## 4.2 The Miraculous Argument

Einstein's light quantum paper (1905a) has nine parts. The last three pertain to empirical vindications of the light quantum hypothesis. Einstein's famous analysis of the photoelectric effect appears in the eighth part only ("On the generation of cathode rays by illumination of solid bodies"). It has such a minor role in the paper that it seems inappropriate to give the paper the moniker, "the photoelectric effect paper." The bulk of the paper, from the first to the sixth sections, is largely devoted to setting up and stating just one argument that comes to fruition in sixth section ("Interpretation of the expression for the dependence of the entropy of monochromatic radiation on volume according to Boltzmann's Principle"). There Einstein infers that the measured thermodynamic properties of high frequency heat radiation carry the distinctive signature of independent, spatially localized points. This argument is, in my view, the most inspired of all Einstein's achievements of 1905 and, for this reason, I have chosen to call it "the miraculous argument."

There were two steps in the argument. The first appeared in the fifth section ("Molecular-theoretical investigation of the dependence of the entropy of gases and dilute solutions on the volume"). It laid out a simple piece of statistical physics. Einstein considered a system consisting of  $n$  independently moving points in a volume  $V_0$  of

space. It followed immediately from the independence of the points that the probability  $W$  that all  $n$  points are located in some subvolume  $V$  is just

$$W = \left(\frac{V}{V_0}\right)^n \quad (4.1)$$

In that same section, Einstein had already presented a brief argument for what he called “Boltzmann’s Principle” (See Section 4.6 below.) That principle

$$S = k \log W \quad (4.2)$$

used Boltzmann’s constant  $k$  to make a connection between the probabilities  $W$  of microstates and their corresponding macroscopic entropies  $S$ . Applying (4.2) to (4.1), Einstein inferred that the entropy change associated with the volume change of (4.1) is

$$S - S_0 = kn \log \left(\frac{V}{V_0}\right) \quad (4.3)$$

In a footnote, Einstein then used standard thermodynamic relations to deduce from (4.3) that the  $n$  points would exert a pressure  $P$  at temperature  $T$  that conforms to the ideal gas law

$$PV = nkT \quad (4.4)$$

The obvious application of these results is to the  $n$  molecules of an ideal gas, which is thereby deduced to conform to the ideal gas law (4.4). The probability  $W$  of (4.1) is the probability that the gas spontaneously fluctuates to a smaller volume  $V$  in the larger volume  $V_0$ . Unless  $V$  coincides almost exactly with  $V_0$ , the probability of these fluctuations for macroscopically sized samples of gas is exceedingly small.

Systems governed by the analysis could be quite different from an ideal gas, however. All that is needed is that the components of the system are independent, spatially localized points. That would be true of molecules of sugar, say, in a dilute solution; or a few, widely spaced small particles suspended in a liquid. All that mattered for the analysis was that these molecules or particles do not interact with each other. That they are in continuous interaction with the surrounding solvent is irrelevant to the deduction of (4.3) and (4.4). As a result it follows immediately that the ideal gas law obtains for the osmotic pressure exerted by a dilute solution. That is true, even though microscopically the solute molecules do *not* move according to the familiar picture of the ideal gas of introductory text books: long periods of free, inertial motion, interrupted briefly by collisions.

Thus far, the analysis was a simple and vivid illustration of basic ideas in statistical physics. The second step of the argument was developed in the following section and was anything but standard. Einstein returned to the measured results concerning heat radiation that he had reviewed in earlier sections. From these results, he inferred the volume dependence of the entropy of a quantity of high frequency heat radiation. That is, if a quantity of heat radiation of fixed energy  $E$  and definite frequency  $\nu$  occupies volume  $V$  or  $V_0$ , then the corresponding entropies  $S$  and  $S_0$  are related by<sup>2</sup>

$$S - S_0 = k \left(\frac{E}{h\nu}\right) \log \left(\frac{V}{V_0}\right) \quad (4.5)$$

---

<sup>2</sup>I have modified the expression of Einstein’s formula notationally by replacing a constellation of constants of Einstein’s formula by the modern  $h$ .

Einstein then used Boltzmann's principle (4.2) to invert the inference from (4.1) to (4.3). It now followed that there is a probability  $W$  satisfying

$$W = \left( \frac{V}{V_0} \right)^{\frac{E}{h\nu}} \quad (4.6)$$

Einstein immediately noted that this probability was just like the probability of the process of spontaneous volume fluctuations of  $n$  independent, spatially localized points, where

$$n = \frac{E}{h\nu} \quad (4.7)$$

That is, it was as *if* the energy  $E$  of the heat radiation had been divided into  $n$  independently moving, spatially localized points of size  $h\nu$ . Preserving the “as if” qualification, Einstein then gave the most cautious and complete statement of the light quantum hypothesis of the paper:

Monochromatic radiation of low density behaves—as long as Wien's radiation formula is valid [i.e. at high values of frequency/temperature]—in a thermodynamic sense, as if it consisted of mutually independent energy quanta of magnitude  $[h\nu]$ .

The “as if” qualification was only a temporary caution. It was dropped in other statements of his conclusion elsewhere in the paper, now taken against the full background of the other experimental results offered as vindicating the light quantum hypothesis.<sup>3</sup>

While Einstein passed immediately from the formula (4.6) to the light quantum hypothesis, two tacit assumptions were needed for the inference. First, the entropies  $S$  and  $S_0$  of expression (4.5) were deduced for systems of radiation in equilibrium. Einstein now tacitly assumed that that the change of entropy (4.5) would obtain also for transitions to non-equilibrium states such as when a volume  $V_0$  of heat radiation fluctuates to a non-equilibrium state with a smaller volume  $V$ .<sup>4</sup>

Second, Einstein tacitly assumed that just such a fluctuation process was possible in which the volume  $V_0$  would spontaneously contract to the small  $V$  in such a way that the system's energy  $E$  and high frequency  $\nu$  would remain unchanged. The constancy of the energy  $E$  was assured by the conservation of energy for an isolated system. However it is not so clear what justifies the assumption of the constancy of the frequency.

This last assumption can easily pass unnoticed if one already has in mind that the system of radiation consists of many non-interacting quanta, each with a characteristic frequency parameter  $n$ . But having that in mind is to anticipate the conclusion, whereas the goal is to infer this conclusion. Minimally one can say that the assumption of constancy of frequency entails the evidence of the observed entropy change and, by virtue of that entailment, the constancy is inductively supported by the evidence. What

<sup>3</sup>For example, in the introduction to the paper Einstein writes that the full constellation of evidence assembled in the paper “seems to be understood better through the assumption that the energy of light is distributed discontinuously in space” and that light propagating from a point source “consists of a finite number of energy quanta, that are localized at points in space, move without dividing and can only be absorbed or produced as a whole.”

<sup>4</sup>For further discussion of this assumption, see Norton (2006, p. 87, n. 15), where it is suggested that the essential condition is that the descriptions of the equilibrium and non-equilibrium macrostates states delimits the same volume of phase space.



would be better is if there was independent support for the assumption. That may be hard to secure. The dynamical laws of the system govern how its frequency will change over time. The whole point of Einstein's argument is to establish that these dynamical laws are not Maxwell's equations; or perhaps that these equations hold at best for the averages of quantities.<sup>5</sup> The fluctuation process is a deviation from average behavior, so we do not know what those dynamical laws are. The presumption that these laws involve quanta that preserve their frequency parameters over time if they are non-interacting is, once again, to anticipate the conclusion sought.

### 4.3 A Familiar Project

What Einstein achieved with his miraculous argument was an inference from the macroscopic properties (the volume dependence of entropy of high frequency thermal radiation) of a thermal system to its microscopic constitution (independent, spatially localized energy quanta). This sort of project was quite familiar to Einstein. It has been the repeated theme of much of his work in statistical physics of 1905 and earlier. His doctoral dissertation (Einstein 1905b) was devoted to inferring from the macroscopic properties of dilute sugar solutions (viscosity, diffusion) to an essential element of their microscopic constitution (size of sugar molecules). In his Brownian motion paper (Einstein 1905c), he established that the predicted<sup>6</sup>, microscopically visible motions of suspended particles result from collisions with moving water molecules and thus would provide a visible manifestation of these last motions. The profound importance of this result was that Einstein had found an effect that could not be treated by equilibrium thermodynamics. Thermodynamicists could no longer ignore the molecular kinetic program if they were to account for the visible motions of suspended particles Einstein now predicted.

The overall project was the same in Einstein's first two publications (Einstein 1901, 1902). These papers now attract little attention in history of science. That conforms with Einstein's own judgment that they are "worthless beginner's works," as expressed to Johannes Stark in a letter of December 7, 1907 (*Papers*, Vol. 5, Doc. 66). A result of this neglect is that it is easy to overlook the continuity in Einstein's projects that extends back to these earliest papers. The goal of these early papers was to develop an hypothesis on the forces between molecules. Einstein had hypothesized that the force between two molecules separated by a distance  $r$  is generated by a potential  $P$  satisfying

$$P = P_{\infty} - c_1 c_2 \varphi(r) \quad (4.8)$$

where  $P_{\infty}$  is the potential when the molecules are infinitely far apart, constants  $c_1$  and  $c_2$  are characteristic of the two molecules and  $\varphi(r)$  is a universal function. Einstein's goal in these papers was to test this hypothesis and to determine values of the constants  $c_1 c_2$ . In the first of these two papers (1901), Einstein sought to infer these microscopic quantities from macroscopic properties of capillarity. In the second (1902), Einstein

---

<sup>5</sup>This possibility is suggested by Einstein's remark in the introduction to the paper that optical experiments on diffraction, reflection, refraction, dispersion, etc. pertain only to the time averages of quantities.

<sup>6</sup>Einstein (1905c) suggested in the introduction to the paper that these motions may be Brownian motion but lamented that the data available to him on Brownian motion was too imprecise for him to know.

replaced macroscopic properties of capillarity with electrochemical potentials known through investigations in electrolysis.

Much of Einstein's earlier and contemporary work was devoted to the project of inferring microscopic constitutions from macroscopic properties. So he had become familiar and quite adept at this project. There was a closer similarity to the project of Einstein's light quantum proposal, as we shall see in the following section.

#### 4.4 Signatures of Many, Independent, Spatially Localized Points

The central idea of Einstein's miraculous argument can be encapsulated in a single, powerful idea. Sometimes it is possible to see a signature of the microscopic constitution of a thermal system in its macroscopic thermodynamic properties. Einstein had identified just such a signature for systems consisting of independent, spatially localized components. That signature is given as the dependence of entropy on the logarithm of volume as expressed in equation (4.3). If that dependency can be identified, then we have a strong indication that the system consists of independent, spatially localized components; the number of components  $n$  can be read directly from the constant of proportionality of (4.3), which is just  $kn$ .

There was, it turns out, a much more familiar (but slightly less powerful) signature of this same microscopic constitution. It is the ideal gas law itself. If one has a system of many, independently moving points, microscopically speaking, they will tend to scatter due to their random thermal motions. This tendency can be redescribed macroscopically as a pressure exerted by the system. It is the ordinary pressure of an ideal gas or the osmotic pressure of dilute solutions.

Well before 1905, it was well known that this relationship could be used as a bridge to pass from the macroscopic observables of a system to its microscopic constitution. To mention one important example, Arrhenius (1887) had used it as a means of inferring the degree of dissociation of solutes in solution. Take, for example, a binary solute. If it is fully dissociated in solution, there will be twice as many components in the solution as there would be if the solute were completely undissociated. That means the osmotic pressure of the fully dissociated solute would be twice that of a completely undissociated solution. As a result, the degree of dissociation of the solute could be determined simply by measuring the osmotic pressure and determining its location between the two extremes.

This ideal gas law and its microscopic underpinnings was an essential component of Einstein's analysis of the diffusion of sugar in his dissertation and of the scattering of small particles in the Brownian motion paper. He used it to deduce an equation important to the analysis of both papers. That equation related the diffusion coefficient  $D$  of systems of sugar molecules or suspended particles, a macroscopic measure of their tendency to scatter, with microscopic quantities, including the radius  $S$  of the molecule or particle<sup>7</sup>

$$D = \left( \frac{RT}{6\pi\eta} \right) \left( \frac{1}{NS} \right) \quad (4.9)$$

<sup>7</sup> $N$  is Loschmidt's (Avogadro's) number;  $R$  is the ideal gas constant;  $\eta$  is the viscosity of the suspending fluid.

This equation was deduced by considering a solution or system of suspended particles in a gravitational field. Gravity would lead the solute and small particles to fall at a rate limited by the viscosity of the fluid and expressed by Stokes law. Osmotic pressure, as given by the ideal gas law, would scatter the solutes and small particles upward. Since the system is at equilibrium, the two motions must cancel on average. Setting them equal yields (4.9).

The deduction of this result depended upon the ideal gas law holding both for the osmotic pressure of a solute and for the pressure used to model the tendency of suspended particles to scatter. While the former conformity to the ideal gas law was widely accepted, the latter was not. For it suggested that the statistical methods of the molecular kinetic approach should apply to small particles visible under the microscope as well. So, in the second section of the Brownian motion paper, Einstein gave a long and careful demonstration of just how little was needed to deduce the ideal gas law. Essentially one needed only to assume that the components of the relevant system did not interact with each other.<sup>8</sup> Small particles suspended in a fluid satisfied this condition if they are spaced widely enough. All that remained was to use the formalism of statistical physics to re-express this fact about the components in macroscopic terms to recover the ideal gas law.

A simpler version of the inference—not given by Einstein—shows just how direct the connection was. Consider a thermal system of independent, spatially localized components (e.g. solute molecules or small particles suspended in a fluid) in a gravitational field.<sup>9</sup> This system is governed by Boltzmann’s distribution. So the probability  $P(h)$  that a given component is located at height  $h$  is

$$P(h) = \text{constant} e^{\frac{-E(h)}{kT}} \quad (4.10)$$

The essential fact of the independence of the components is expressed in this formula through the fact that the energy  $E(h)$  of each component is a function of height  $h$  only.<sup>10</sup> That is, it is independent of the positions of the other components. It now follows immediately that the density  $\rho$  of components at height  $h$  in relation to its density  $\rho_0$  at height  $h = 0$  is

$$\rho = \rho_0 e^{\frac{-E(h)}{kT}}$$

---

<sup>8</sup>This fact is quite remarkable. That sugar molecules in a dilute solution will be in constant interaction with the molecules of water of the solvent does not affect the recovery of the ideal gas law for the sugar’s osmotic pressure. All that matters is that the sugar molecules do not interact with each other, a condition enforced by the diluteness of the solution.

<sup>9</sup>The standard technique for introducing osmotic pressure in the literature had been through the force exerted by some species of a solute on a semi-permeably membrane, that is, a membrane permeable to everything but the molecules of that species of solute. In his (1902), Einstein had expressed doubts over whether such membranes are realistic. With great care, he proposed that osmotic pressures are better analyzed by equilibration with conservative fields that would act differentially on the different species of solute molecules. This technique enables the greatly simplified and generalized derivation of the ideal gas law presented here. Einstein introduced the technique casually in both his dissertation and his Brownian motion paper without giving a citation to his earlier, careful analysis of it. This is another example of Einstein’s laxity in citing his sources, yet in this case it was his own earlier work that was obscured.

<sup>10</sup>It is assumed that the total energy is a sum  $E = E(h) + E_{KE}$ , where  $E_{KE}$  is the component’s kinetic energy. The kinetic energy will contribute a term to (4.10) that is absorbed into the constant

The density gradient due to gravitational field can be found by differentiating this expression with respect to  $h$

$$\frac{d\rho}{dh} = -\frac{1}{kT} \frac{dE}{dh} \rho$$

This equilibrium density gradient arises from a balancing of two forces. The first is the gravitational force density

$$f = -\frac{dE}{dh} \rho$$

acting on the components in the downward direction. It is balanced by the pressure  $P$  that arises from the tendency of the components to scatter. Components will be accelerated whenever there are neighboring regions of different pressure. The resulting force  $f$  is given by the pressure gradient

$$f = \frac{dP}{dh}$$

Combining, the expression for the density gradient becomes

$$\frac{d\rho}{dh} = -\frac{1}{kT} \frac{dE}{dh} \rho = \frac{1}{kT} f = \frac{1}{kT} \frac{dP}{dh}$$

Rearranging the terms, we recover

$$\frac{d}{dh}(P - \rho kT) = 0$$

Integrating with the boundary condition that  $P = 0$  when  $\rho = 0$  yields a local form of the ideal gas law

$$P = \rho kT$$

When the component distribution is sufficiently homogeneous that it can be represented as  $n$  components spread uniformly over a volume  $V$ , we have  $\rho = n/V$  and the ideal gas law adopts its extended form

$$PV = nkT$$

This demonstration shows clearly that the ideal gas law is little more than a macroscopic re-expression of the microscopic fact of independence of spatially localized components. Its simplicity strongly suggests that the inference may be inverted: when we have a system of components obeying the ideal gas law, we can infer that they are independent, spatially localized components. The inference can be so inverted, although the details are a little messy.<sup>11</sup> Thus the ideal gas law can function as a signature of the microscopic constitution of a system, although, as we shall see in the next section, it proves to be a little less revealing than Einstein's entropy-volume relation (4.3).

## 4.5 Why Didn't Einstein Use the Ideal Gas Law as the Signature?

The results of the last section raise a question. Why did Einstein need to discover a new macroscopic signature of the microscopic constitution of independent, spatially localized

---

<sup>11</sup>See *Norton* (2006, Appendix A "The Ideal Gas Law").

components? The ideal gas law is a long-standing, widely appreciated signature of just such a constitution; one that would be understood more easily by his readers of 1905; and one that Einstein was so familiar with, that his other work of 1905 included a thorough analysis of it.

There is one easy answer to the question that does not bear scrutiny. One might imagine that the ideal gas law fails for high frequency heat radiation. For the simplest application of the ideal gas law is to an isothermal expansion of a gas. In such a process the gas pressure  $P$  varies inversely with the volume  $V$ ; this specialization of the ideal gas law is Boyle's law

$$PV = \text{constant} \quad (4.11)$$

This result does not obtain for heat radiation, however. It is a familiar property of heat radiation that the pressure  $P$  it exerts is a function solely of the energy density  $u$

$$P = \frac{u}{3} \quad (4.12)$$

The energy density  $u$  is, in turn, a function of the temperature and frequency only; or it is a function of the temperature only, if we consider full spectrum heat radiation. So, in an isothermal expansion of full spectrum heat radiation, the pressure  $P$  will stay constant precisely because the process is isothermal and has a fixed temperature.

This constancy of pressure in an isothermal expansion does not establish the failure of the ideal gas law for heat radiation. The inference to the failure is flawed since it does not take into account an essential disanalogy between ideal gases and heat radiation. For an ideal gas, the number of components, that is, the number of molecules, remains constant during an isothermal expansion. For heat radiation, however, the number of components does not remain constant during an isothermal expansion. Indeed this process will create new quanta. The total energy  $E = uV$ . Since  $u$  stays constant in the process and  $V$  increases, it follows that the system's total energy  $E$  must increase and, with it, the total number of quanta also increases.<sup>12</sup> This means that the relevant specialization of the ideal gas law to the isothermal expansion of heat radiation is not Boyle's law (4.11), but one that retains dependency on  $n$

$$PV = \text{constant } n$$

This extended form of Boyle's law obtains for the isothermal expansion of ideal gases and also, as we shall see in a moment, for high frequency heat radiation as well. Where they differ is in how  $P$  behaves during the expansion. For an ideal gas, since  $n$  is constant, pressure  $P$  will decrease in inverse proportion to  $V$ . For high frequency heat radiation, the number of quanta  $n$  will grow in direct proportion to the volume  $V$ ; the result is that  $P$  remains constant during the process.

So far, we have only seen that consideration of isothermal expansions do not give *prima facie* grounds for expecting the ideal gas law to fail for heat radiation. That does not establish that the ideal gas law does obtain for heat radiation. The ideal gas law does indeed obtain for high frequency heat radiation, although to see it requires a result from Einstein's 1905 light quantum paper. In Section 6 of that paper, Einstein computed

---

<sup>12</sup>Contrast this with the familiar property of ideal gases, that their total energy remains constant during an isothermal expansion.

the mean energy of quanta for radiation governed by Wien's distribution law. That law obtains for high frequency radiation, so Einstein's result holds as long as we consider only high frequency radiation. He found that the mean energy of these quanta is  $3kT$ , so that the energy density  $u = 3nkT/V$ . Combining this with the expression (4.12) for radiation pressure, we find

$$P = \frac{u}{3} = \frac{(3nkT/V)}{3} = \frac{nkT}{V}$$

which is just the ideal gas law.<sup>13</sup> Now we can return to the question posed at the start of this section. The ideal gas law does obtain for heat radiation and was then a familiar signature of a microscopic constitution of many, independent components. So why didn't Einstein use it in his light quantum paper? Einstein gave no answer to this question. However even a cursory perusal of how the corresponding argument would run shows that it would be quite unconvincing as a means of establishing the existence of quanta. For high frequency radiation governed by Wien's distribution, the energy density  $u$  of radiation would conform to the familiar Stefan-Boltzmann law  $u = \sigma T^4$ . Substituting this into the expression for radiation pressure (4.11) we recover

$$P = \frac{u}{3} = \frac{\sigma T^4}{3} = \left( \frac{\sigma VT^3}{3k} \right) k \frac{T}{V} = \frac{nkT}{V}$$

To complete the argument, we would need to proclaim that the number of quanta can be read from the last equality as

$$n = \frac{\sigma VT^3}{3k}$$

That would be a quite unconvincing proclamation to someone who has no allegiance to the notion of the light quantum and may even have never conceived it. The equality makes clear that the number of quanta will vary in most familiar thermodynamic processes. We see that the number of quanta  $n$  will increase in direct proportion to the volume  $V$ , as noted before. The number of quanta  $n$  will also increase with the cube of temperature. One would be forgiven for thinking that these components are rather unlike the permanent gas molecules, solute molecules and suspended particles of the familiar applications of the ideal gas law. These quanta are created and destroyed by expansion and compression and by heating and cooling. Indeed, if one is unsure of the number of components in a thermal system, the ideal gas law is not a reliable signature of their constitution. That is, the mere proportionality of  $PV$  with  $kT$  for some thermal system does not assure us that the constant of proportionality is the number of spatially localized components.<sup>14</sup> However if we know the number of components so that we supply the " $n$ " of  $pV = nkT$ , the obtaining of the ideal gas law does allow us to infer their independence and spatial localization.

Since Einstein had no independent indication of the number of components in high frequency heat radiation, he needed a different signature; and ideally it would be one that does not draw attention to the tenuous existence of light quanta. Such a signature should be sought in processes that leave the number of quanta fixed. There are very few such

<sup>13</sup>The ideal gas law also turns out to obtain if we consider a single frequency cut of high frequency heat radiation, although the calculation is more difficult. For details, see *Norton* (2006, p. 91).

<sup>14</sup>For an illustration of how the inference can fail, see *Norton* (2006, p. 77–78)

processes. Heating, cooling and the normal sorts of volume changes all alter the number of quanta. What Einstein managed to locate in the process of volume fluctuations is a process, rare among those treated by the thermodynamics of heat radiation, that turns out not to alter the number of quanta. As a result, it proves especially hospitable to the signature Einstein employed of the dependence of entropy on the logarithm of volume. Moreover he did not need to know in advance how many components comprised the system under investigation. Once the proportionality of entropy and the logarithm of volume was ascertained, the number of components could be read from the constant of proportionality.

Finally, it should be noted that this signature of the dependence of entropy on the logarithm of volume is much harder to see in heat radiation than in the case of ideal gases. In the case of ideal gases, the two states that are related by the probability formula (4.1) can also be connected by an isothermal compression. That means that the dependence of entropy on the logarithm on volume is a familiar result from studies of the processes of equilibrium thermodynamics. That is not the case for heat radiation. Unlike the case of an ideal gas, an isothermal compression of a system of heat radiation will change the system's energy. It follows that this process is not governed by the entropy-volume relation (4.3) that is central to Einstein's argument. More complicated processes, such as the volume fluctuation process Einstein described, are needed to connect the two states.

## 4.6 Einstein's Demonstration of Boltzmann's Principle

The considerations developed here help us understand the role played by a famous demonstration Einstein included in Section 5 of his light quantum paper. There Einstein sought to lay out a general argument for what he called "Boltzmann's principle," which is expressed in the iconic formula " $S = k \log W$ " rendered as (4.2) above.

The argument begins by considering two independent thermal systems with probabilities  $W_1$  and  $W_2$ . Because the systems are independent, the probability of the joint system is simply given by the product

$$W = W_1 W_2 \tag{4.13}$$

Now, Einstein continued, entropy  $S$  is a function of  $\varphi(W)$  of probability and, since entropy is an extensive magnitude, the entropy  $S$  of the joint system must be the sum of the entropies  $S_1$  and  $S_2$  of the two component systems

$$S = S_1 + S_2 \tag{4.14}$$

It is a simple problem in functional analysis to verify that the only function  $S = \varphi(W)$  satisfying these two conditions (4.13) and (4.14) is

$$S = \text{constant} \log W \tag{4.15}$$

where the constant of this relation must be Boltzmann's constant  $k$  if the relation is to conform with other results in the kinetic theory of gases.

It is hard not to be dazzled by this argument. It requires only the simplest of analyses to deliver a beautifully simple explication of entropy, the most contentious notion in statistical physics. Yet the argument is also quite maddening. For, in its speedy execution, it passes in silence over a series of important questions:

- What are the probabilities of equation (4.13)? The probability of an outcome has no clear meaning if we do not specify an outcome space and the conditions governing it. We cannot speak without fatal ambiguity of the probability that a coin shows a head if we do not also specify that we have a fair coin with a head on one side and a tail on the other and that it is flipped in a fair toss.
- To arrive at the simple formula (4.15), Einstein must assume that entropy  $S$  is a function of probability only. Otherwise the constant of the formula is constant only with respect to probability; we have not ruled out the possibility that it is a function of the system's other properties. How do we know that entropy  $S$  is a function of the probability  $W$  only, for all thermal systems, not just for kinetic gases?
- Einstein's argument connects only to the thermodynamic notion of entropy in that it is required in (4.14) that the quantity  $S$  be an extensive magnitude. It is not shown that the resulting  $S$  of  $S = k \log W$  coincides with the thermodynamic entropy of the system as specified in the Clausius definition

$$S - S_0 = \int dq_{rev} \frac{1}{T} \quad (4.16)$$

where  $S$  is the entropy of a system with initial entropy  $S_0$  after a reversible process in which quantities of heat  $q_{rev}$  are imparted to it at temperature  $T$ . At best the argument can establish that, if there is any quantity at all that is a function of probability only that coincides with thermodynamic entropy, then it must be that of (4.15).

Clausius' entropy (4.16) is defined only for equilibrium states. Yet Einstein intends the quantity  $S$  of (4.15) to apply to non-equilibrium states such as are produced by fluctuation processes. Does Einstein have an independent standard that authorizes his assigning the term "entropy" to this quantity? Or is it a definition? If it is a definition, why is it appropriate to continue to assume that the extended notion of entropy now being defined should conform to the additive requirement (4.14)? Perhaps a natural, non-equilibrium notion of entropy is non-additive.

My point here is not to deny Einstein's result. In so far as we now have a serviceable explication of entropy in the modern literature, it equates entropy with  $k$  times the logarithm of volume in phase space; that is the analog of Einstein's  $S = k \log W$ . Rather my point is that Einstein's analysis is hasty in the way it suppresses background assumptions and steps needed to complete the argument.

Einstein certainly knew how to give a more precise analysis of entropy in terms of phase space quantities. It was included in his papers prior to 1905 on the foundations of statistical mechanics. Notably Section 6 of Einstein (1903) used Clausius' definition (4.16) of thermodynamic entropy to ground the expression for the canonical entropy of an equilibrium system at temperature  $T$  and with mean energy in a phase space with canonical coordinates  $p_1, \dots, p_n$

$$S = \frac{\bar{E}}{T} + k \log \int e^{(-\frac{E}{kT})} dp_1 \dots dp_n \quad (4.17)$$



Indeed this result was not far from Einstein's thoughts in 1905. It is recapitulated, along with the statement of the equations of motion governing the system point of the phase space, in Section 2 of the 1905 Brownian motion paper and forms the basis of Einstein's derivation of the ideal gas law.

So why did Einstein regress from the precision of his 1903 analysis of the canonical entropy formula (4.17) to the ambiguity and incompleteness of his 1905 demonstration of Boltzmann's principle? My conjecture is that Einstein regressed to a less precise analysis because the 1903 analysis required presumptions that he knew were either false for light quanta or at least uncertain; and it did not analyze quite the process at issue in 1905.

To elaborate, the 1903 analysis presumed a fixed number of components, in so far as the number of components in the system is equated with the dimension of the phase space. For the 1903 analysis presumed a phase space with  $n$  fixed dimensions and fixed canonical coordinates  $p_1, \dots, p_n$ . Einstein's 1905 system, however, had a variable number of components, in that the number of quanta vary in the course of typical thermodynamic processes.

Next, Einstein's 1903 analysis presumed definite, Hamiltonian-like equations of motion. Einstein's 1905 analysis of light quanta had yielded no equations of motion for individual quanta. At best one could guess what they might be in special cases.<sup>15</sup>

Finally, the 1903 analysis connected the entropy of a system at thermal equilibrium with the corresponding phase space quantities. In 1905, Einstein needed more. It was essential to his miraculous argument that at least one of the states was a non-equilibrium state arrived at by a possibly extremely unlikely fluctuation. In his 1905 analysis of light quanta, Einstein needed to related the entropy of a system with its microscopic constitution in a way that did not rely on a phase space of fixed dimensions, that did not need the presumption of any definite equations of motion and that extended to highly non-equilibrium systems. Einstein argument for Boltzmann's principle met all these demands. In particular, its maddening vagueness is a reflection of the incompleteness of Einstein understanding of quanta. The more precise he made his argument for Boltzmann's principle, the more he risked that the presumptions of his argument might not apply to his target system of light quanta.

## 4.7 Conclusion

Einstein's miraculous argument for light quanta is a fascinating mix of insecurity and security. It was insecure in that the notion of light quanta directly contradicted the proudest achievement of nineteenth century physics, the wave theory of light. It was secure in that the methods used to infer the existence and properties of light quanta were standard techniques of statistical physics, albeit in an inspired variation. I have urged that by 1905 Einstein had become accomplished in inferring the microscopic constitution of systems from their macroscopic properties and that he was especially familiar with systems consisting of many, independent, spatially localized components. Bolstered with the further empirical evidence of the closing three sections of the paper concerning photoluminescence, the photoelectric effect and the ionization of gases, Einstein could

---

<sup>15</sup>For example, free quanta plausibly propagate uniformly in straight lines at the speed of light.

be confident that the light quantum hypothesis was correct. What remained obscure then and later was precisely how the truth of such an extraordinary departure from the wave theory could come about.

I have not advanced any conjectures on the specific historical pathway that Einstein followed to his proposal of the light quantum. However it seems very plausible to me that some role was played by Einstein's familiarity with the macroscopic appearance of systems consisting of many, independent, spatially localized components. It would be interesting to know which signature of discreteness Einstein first found, how early he found it in his conceiving of the light quantum hypothesis and how close it was to the signature actually offered in his 1905 light quantum paper.

## References

- Arrhenius, Svante (1887): "Über die Dissociation der in Wasser gelösten Stoffe," *Zeitschrift für physikalische Chemie* 1, pp. 631–48. Translated as "On the Dissociation of Substances in Aqueous Solution" in M. J. Nye, ed., *The Question of the Atom: From the Karlsruhe congress to the First Solvay Conference, 1860–1911*. Los Angeles: Tomash 1984, pp. 285–309.
- Einstein, Albert (1901): "Conclusions drawn from the phenomenon of Capillarity," *Annalen der Physik* 4 (1901), pp. 513–523.
- Einstein, Albert (1902): "On the thermodynamic theory of the difference in potentials between metals and fully dissociated solutions of their salts and on an electrical method for investigating molecular forces," *Annalen der Physik* 8 (1902), pp. 798–814.
- Einstein, Albert (1903): "Eine Theorie der Grundlagen der Thermodynamik," *Annalen der Physik* 11, pp. 170–187.
- Einstein, Albert (1905a): "On a heuristic viewpoint concerning the production and transformation of light," *Annalen der Physik* 17 (1905), pp. 132–148. (17 March 1905)
- Einstein, Albert (1905b): A New Determination of Molecular Dimensions. Buchdruckerei K. J. Wyss, Bern, 1905; *Annalen der Physik* 19 (1906), pp. 289–305. (30 April 1905)
- Einstein, Albert (1905c) "On the motion of small particles suspended in liquids at rest required by the molecular-kinetic theory of heat." *Annalen der Physik* 17 (1905), pp. 549–560. (May 1905; received 11 May 1905)
- Einstein, Albert (1905d) "On the Electrodynamics of Moving Bodies," *Annalen der Physik* 17 (1905), pp. 891–921. (June 1905; received 30 June, 1905)
- Einstein, Albert (1905e) "Does the Inertia of a Body Depend upon its Energy Content?" *Annalen der Physik* 18 (1905), pp. 639–641. (September 1905; received 27 September, 1905)

Klein, Martin J. et al. (eds.) (1993) *The Collected Papers of Albert Einstein, Volume 5: The Swiss Years: Correspondence, 1902–1914*. Princeton: Princeton University Press. (“*Papers*, Vol. 5”)


Norton, John D. (2006) ”Atoms Entropy Quanta: Einstein’s Miraculous Argument of 1905,” *Studies in History and Philosophy of Modern Physics* 37 (2006), pp. 71–100.

# 5 The Ehrenfest Adiabatic Hypothesis and the Old Quantum Theory, before Bohr

ENRIC PÉREZ CANALS AND MARTA JORDI TALTAVULL

*HQ1-S1*

## The Ehrenfest Adiabatic Hypothesis and the Old Quantum Theory, before Bohr



**Enric Pérez Canals**  
**Marta Jordi Taltavull**  
Universitat de Barcelona

Paul Ehrenfest at University of Leiden

This talk deals with the role of the adiabatic hypothesis in the development of the old quantum theory. This hypothesis was formulated by Ehrenfest in a paper published in 1916, but practically all the results that appeared there had been published by him during the previous ten years. What Ehrenfest did in 1916, was to collect all those earlier results on the adiabatic transformations and their relations to the quantum theory, with the idea that they should become widely known. Far from that, the Ehrenfest's 1916 paper had little impact during the next few years. It was only after Bohr in 1918 published an essential work about the quantum theory, where he used the adiabatic hypothesis, that its importance began increasing.

To sum up the role that the adiabatic hypothesis played in the development of the old quantum theory up to 1918, what follows is centred in these four axes:

1. Summary of the antecedents of the Ehrenfest's adiabatic hypothesis (1905–1914).
2. Description of the main contents of the Ehrenfest's 1916 paper.
3. Analysis of the first responses, before the publication of the Bohr's work in 1918.
4. Commentaries on the role of the adiabatic hypothesis in the Bohr's work.

Outline

1. Antecedents of the Ehrenfest's adiabatic hypothesis (1905 -1914).
2. "On adiabatic changes of a system in connection with the quantum theory" (1916).
3. First reactions (1916-1918).
4. The adiabatic hypothesis in 1918 Bohr's paper.

### **Antecedents of Ehrenfest's Adiabatic Hypothesis (1905–1914)**

Paul Ehrenfest was born in 1880 in Vienna, where he carried out his studies in Physics and Chemistry, and became a doctor in 1904 under the guidance of Boltzmann. That is why it is not strange that one of his principal interests was statistical mechanics.

In 1905, Ehrenfest published his first paper on quantum theory (see slide  $S_3/1$ ). However, it would not be until the paper published one year later that he clearly adopted a statistical approach to the quantum theory. In both papers, he criticized Planck's theory of black-body radiation.

## Ehrenfest towards the adiabatic hypothesis, I (1905-1911)

- **1905-1906: Criticism of Planck's theory of black-body radiation.**
  - **1905:** "Über die physikalischen Voraussetzungen der Planck'schen Theorie der irreversiblen Strahlungsvorgänge". *Akademie der Wissenschaften, Vienna. Sitzungberichte. Abteilung II*, 1301-1314.
  - **1906:** "Zur Planckschen Strahlungstheorie". *Physikalische Zeitschrift* 7, 528-532.

Anyway, at that time, Ehrenfest's statistical tools were only insinuated. It was in the ensuing years that he would develop them in his notebooks. With the paper of 1911 being the cornerstone of his work, for there he carries out a statistical analysis of the radiation (see slide  $S_3/2$ ). It is important to highlight some points of this crucial publication that specially concern our purposes in this brief exposition:

- Ehrenfest proved that by imposing the validity of Boltzmann's principle,

$$S = k \log W$$

( $S$  is the entropy,  $k$  Boltzmann's constant, and  $W$  the probability of a macrostate), Wien's displacement law could be obtained.

- In the corresponding proof, Ehrenfest imposed that the variation of the entropy was zero during an adiabatic compression of the cavity that contained the radiation (in an adiabatic compression the work done completely turns into energy of the system). Here Ehrenfest took advantage, for the first time, of an adiabatic invariant, which is a quantity that remains constant during this type of transformations. In the case of the radiation in a cavity, the invariant quantity is:

$$\frac{E_\nu}{\nu},$$

where  $E_\nu$  is the energy of a mode of vibration, and  $\nu$  its frequency.

- By following this procedure, he also discovered that, in order to account for some indisputable features of the spectral distribution law, the quantization might be applied precisely to the adiabatic invariants, so justifying the form of the Planck's quantum of energy, as any other quantization would have contradicted Boltzmann's law ( $h$  is Planck's constant):

$$\frac{E_\nu}{\nu} = 0, h, 2h, 3h, \dots$$

HQ1-S3/2

- **1907-1911: Statistical analysis of radiation.**
  - 1911: "Welche Züge der Lichtquantenhypothese spielen in der Theorie der Wärmestrahlung eine wesentliche Rolle?". *Annalen der Physik* 36, 91-118.
  - By imposing  $S = k \log W$ , he obtains Wien's displacement law.
  - He uses the adiabatic invariant  $\frac{E_\nu}{\nu}$ .
  - He proves that the quantization must be applied to the adiabatic invariant  $\frac{E_\nu}{\nu} = 0, h, 2h, 3h, \dots$

In 1912, Ehrenfest tried to extend these results to more general mechanical systems. This research gave rise to two papers in 1913.

HQ1-S4/1

## Ehrenfest towards the adiabatic hypothesis, II (1912-1914)

- **1912-1913: Extension of the 1911 results to any periodic motion.**
  - 1913: "Bemerkung betreffs der spezifischen Wärme zweiatomiger Gase". *Verhandlungen der Deutschen Physikalischen Gesellschaft* 12, 451-457.
  - 1913: "A mechanical theorem of Boltzmann and its relation to the theory of energy quanta". *Proceedings of the Amsterdam Academy* 16, 591-597.
- **Connection between allowed motions of different systems.**

In the first one, Ehrenfest deduced the quantization of the energy of a system of rotating molecules, by using an adiabatic transformation. To analyze it, Ehrenfest:

- considered a quantized system of harmonically vibrating electric dipoles in the presence of a strong orienting field (the dipole behaves like a Planckian resonator);

## The Ehrenfest Adiabatic Hypothesis and the Old Quantum Theory

---

- after diminishing the value of the orienting field adiabatically, from a finite number to zero, saw that, as in this last state the electric dipoles did rotate, it was possible to connect adiabatically the vibration and the uniform rotation, and stated that the allowed quantum motions became (other) allowed quantum motions after an adiabatic transformation;
- and with this, he could deduce, as he knew the quantization of the energy for the vibrating molecules, thanks to the quantization of the adiabatic invariant at this point, the quantization for the rotating molecules.

This is the germ of the adiabatic hypothesis, although in this paper Ehrenfest scarcely justified it. It was in the second work of 1913, where he fully justified that supposition. In all likelihood, this is the work that contains the earliest version of the adiabatic hypothesis, although Ehrenfest did not call it this way.

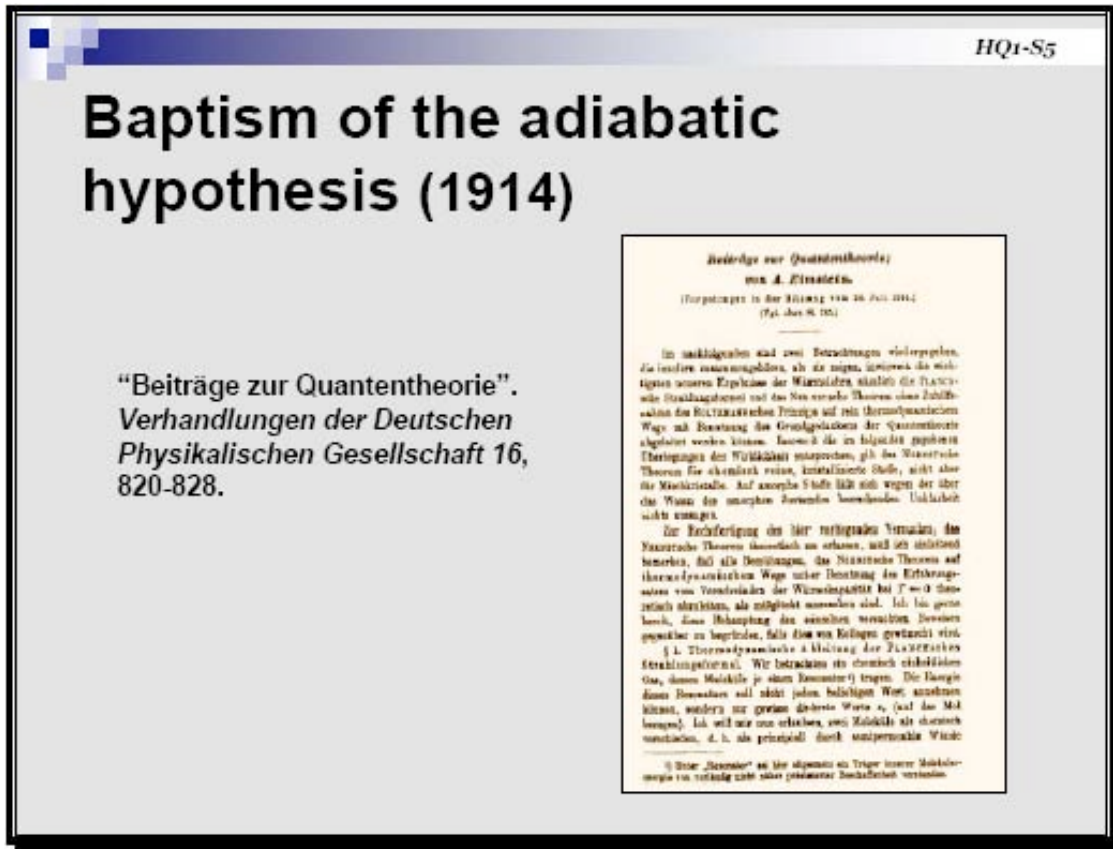
We cannot dwell upon this point, but it must be pointed out that in this stage of his research, Ehrenfest did think that the quantization of the adiabatic invariant was compatible with the validity of Boltzmann's principle. In fact, in the 1911 paper he got to Wien's displacement law and also to the necessity of quantizing the adiabatic invariants by imposing, among other things, Boltzmann's principle. But later research, started by Ehrenfest in the summer of 1913, led him to realize that this compatibility may not be so obvious. So in 1914 he opened another line of investigation to see in which cases would Boltzmann's statistical foundations of the second law of thermodynamics be valid (see slide S4/2). Ehrenfest could not obtain a definitive result, but he could prove that the previous uses of Planck's, Debye's, and Einstein's of this principle were valid.

HQ1-S4/2

• 1914: **Inquiries on the validity of Boltzmann principle:  $S = k \log W$**

• 1914: "Zum Boltzmannschen Entropie-Wahrscheinlichkeits-Theorem".  
*Physikalische Zeitschrift* 15, 347-352.



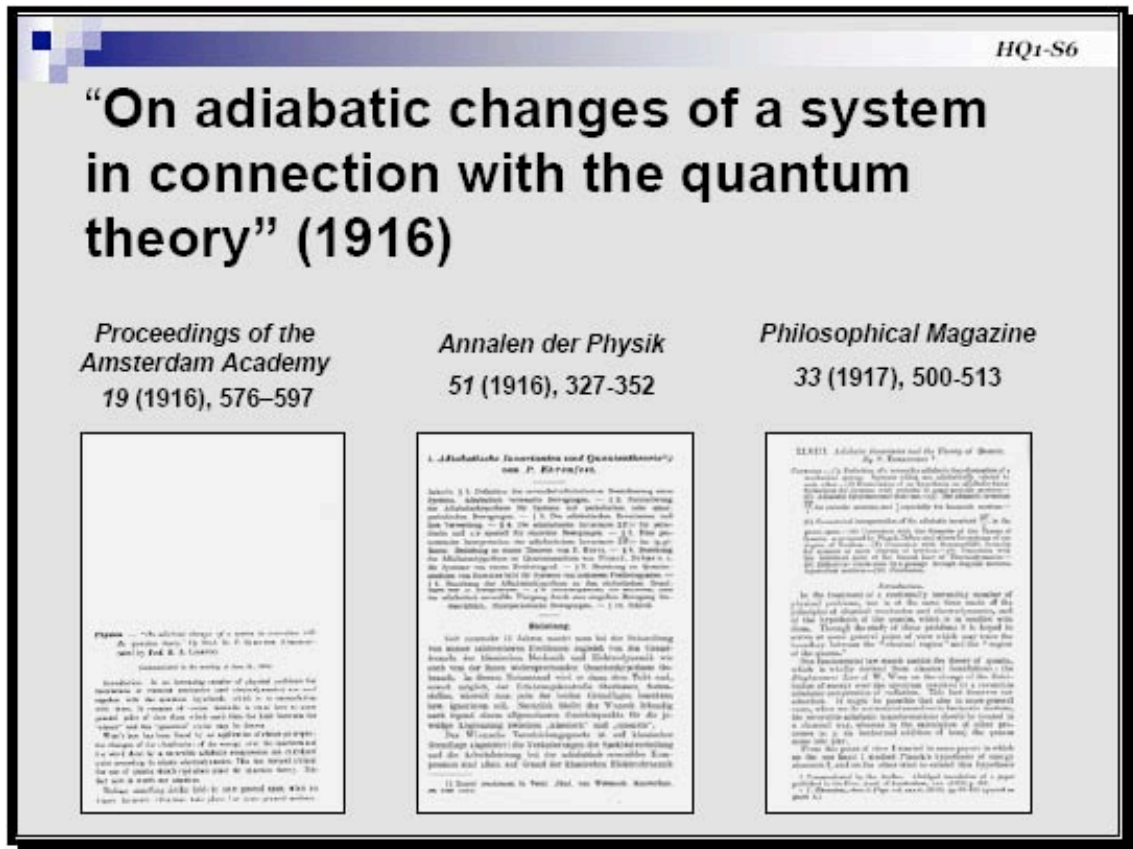


Ehrenfest did not call the adiabatic hypothesis this way in 1914, it was Einstein who did, and used it for the first—and, as far as we know, last—time in his quantum researches in a paper published in 1914. This paper—that contains an erroneous application of the hypothesis—was consequence of an intense dialogue that these two friends kept in the first months of 1914 about the adiabatic idea.

Apart from this Einstein’s contribution, the results obtained by Ehrenfest had no visible incidence whatsoever during the next few years. Not even Sommerfeld nor Planck would worry about proving the compatibility of their respective quantum rules of 1915 with the adiabatic hypothesis. Probably compelled by this ignorance, Ehrenfest decided to gather all his previous results in a new paper and publish it in three different journals, as he thought that the adiabatic hypothesis should furnish with a basis on which to generalize the quantum theory.

### “On Adiabatic Changes of a System in Connection with the Quantum Theory” (1916)

These are the front pages of the three versions of the paper written in 1916, which are practically the same (we will quote the version of *Philosophical Magazine*):



The main contents are the following:

1. Formulation of the hypothesis.
2. Its relation to other quantum rules. This being the principal novelty respect to prior Ehrenfest's results. At this point he shows that his hypothesis agrees with the quantization rules proposed by Planck, Sommerfeld, and Debye.
3. Examination of some difficulties that appear in the application of the hypothesis: the singular motions.
4. Connection between the adiabatic hypothesis and the statistical interpretation of the second law of thermodynamics.

In this new presentation, Ehrenfest calls the hypothesis by its name, and offers an accurate formulation of it. Moreover, contrary to the 1913 papers, the way of presenting the results is systematic. Let's see shortly its contents, bearing in mind that this is the most complete version that Ehrenfest gave of his hypothesis.

The slide features a blue header with the text 'HQ1-S7' in the top right corner. The main title is '“On adiabatic changes of a system in connection with the quantum theory” (1916)'. Below the title is a white box with a black border containing the word 'Contents:' followed by a numbered list of four items.

### Formulation of the Hypothesis

Before the formulation, Ehrenfest defines a “reversible adiabatic affection of a system”. To do that, he considers:

- A potential energy that depends on the coordinates  $q_1, q_2, \dots$ , and on certain parameters  $a_1, a_2, \dots$  “the values of which can be altered infinitely slowly”.
- A kinetic energy  $T$ , which is an homogeneous quadratic function of the velocities  $\dot{q}_1, \dot{q}_2, \dots$ , and the coefficients of which are functions of  $q_1, q_2, \dots$ , and may be of  $a_1, a_2, \dots$

Ehrenfest defines a reversible adiabatic influence on a system as an infinitively slow change of the parameters  $a_1, a_2 \dots$

HQ1-S8/1

## Formulation of the hypothesis

**Reversible adiabatic influence on a system:**

- Potential energy depends on the coordinates  $q_1, q_2, \dots$  and slowly changing parameters  $a_1, a_2, \dots$
- Kinetic energy  $T$  is an homogeneous quadratic function of the velocities. Its coefficients are function of  $q_1, q_2, \dots$  and  $a_1, a_2, \dots$

motion  $\beta(a_1)$ 
➔
motion  $\beta(a_1')$

Infinitesimal slow change of the parameter  $a_1$

Given this definition, Ehrenfest enunciates his hypothesis:

HQ1-S8/2

*For general values  $a_1, a_2, \dots$  of the parameters, those and only those motions are allowed which are adiabatically related to the motions which were allowed for the special values  $a_{10}, a_{20}, \dots$  (i.e. which can be transformed into them, or may be derived from them in an adiabatic reversible way).*

This perfectly fits what Ehrenfest had supposed in his first paper of 1913, when he deduced for the first time the quantization of the energy of a system of rotating dipoles, by using an adiabatic transformation.

It is obvious that the adiabatic invariants play a very important role in this procedure. Ehrenfest referred to them in this way:

HQ1-S9/1

## Adiabatic invariants

*If an adiabatic invariant  $\Omega$  for the 'allowed' motions  $B\{a_0\}$ , belonging to the special values  $a_{10}, a_{20}, \dots$ , possesses the distinct numerical values  $\Omega', \Omega'', \dots$ , it possesses exactly the same values for the 'allowed' motions belonging to arbitrary values of the parameters  $a_1, a_2, \dots$*

This statement implies that quantum rules must be enunciated through these quantities, because they must characterize the allowed motions.

As an example of an adiabatic invariant, Ehrenfest gives one for periodic motions, obtained from a mechanical theorem of Boltzmann's, Clausius', and Szily's, which is:

$$\delta' \int_0^P 2T dt = 0$$

( $\delta'$  stands for the variation during an adiabatic transformation;  $P$  is the period of the motion, and  $T$  the kinetic energy). From this theorem, Ehrenfest obtains the following adiabatic invariant:

$$\frac{2\bar{T}}{\nu}$$

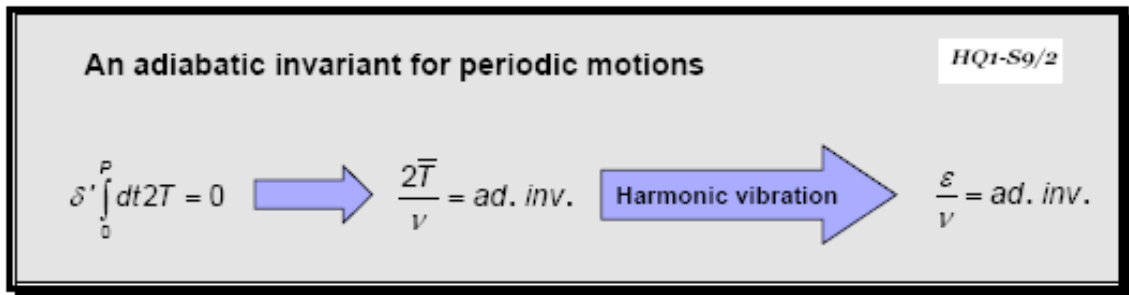
( $\nu$  is the frequency of the motion, and  $\bar{T}$  the mean value of the kinetic energy during a period). Moreover, in the case of harmonic vibration, this invariant becomes:

$$\frac{\epsilon}{\nu}$$

( $\epsilon$  is the total energy, that is, the kinetic and the potential ones), being this expression perfectly related to Planck's quantization of energy done in 1900:

$$\frac{\epsilon}{\nu} = 0, h, 2h, 3h, \dots$$

Summarizing:



### Relation to Quantum Rules

To connect his hypothesis with Planck's and Debye's quantization rules, Ehrenfest proposed an example referred to a one-dimensional system that consisted of a non-linear oscillator. By imposing  $a_1 = a_2 = 0$  (see slide  $S_{10}$ ), it is possible to recover the equation of motion of an harmonic oscillator, i.e., of a Planck's resonator. In this case, the potential energy curve is a parabola, and the allowed motions describe ellipses on the phase plane.

HQ1-S10

## One-dimensional systems

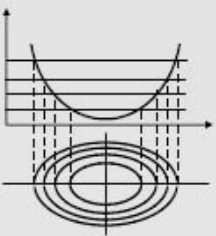
Resonator with a non-linear equation of motion:

$$\ddot{q} = -(\nu_0^2 q + a_1^2 q^2 + a_2^2 q^3 + \dots)$$

If  $a_1 = a_2 = \dots = 0$ :

$$\frac{\varepsilon}{\nu_0} = \frac{2T}{\nu_0} = \iint dqdp = 0, h, 2h, \dots$$

Planck's resonator

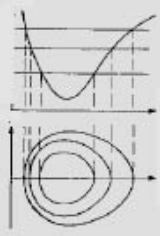


Adiabatic  
transformation  
→

If  $a_1 \neq a_2 \neq \dots \neq 0$ :

$$\frac{\varepsilon}{\nu} = \frac{2T}{\nu} = \iint dqdp = 0, h, 2h, \dots$$

Debye's anharmonic oscillator



Reversing the reasoning, by considering an adiabatic change of the value of the parameters  $a_1, a_2 \dots$  from zero to any finite value, we can see how the equation of motion that it is obtained corresponds to an anharmonic oscillator. According to Debye's quantization, the allowed motions are defined by the closed curves represented on the corresponding phase plane, which are quite different from those of Planck's. As the quantities that remain constant during an adiabatic transformation are the quantities on which the quantization must be applied, both quantization rules, Planck's and Debye's, have to be equivalent to Ehrenfest's adiabatic hypothesis.

To connect his hypothesis with the Sommerfeld quantization rules, Ehrenfest considers a central system that can be described by the following equations of motion:

HQ1-S11/1

## More than one degree of freedom

Potential of central attracting force in polar coordinates:

$$\left. \begin{aligned} m\ddot{r} - mr\dot{\phi}^2 + \frac{d\chi}{dr} &= 0 \\ \frac{d}{dt}(mr^2\dot{\phi}) &= 0 \end{aligned} \right\} \text{As } mr^2\dot{\phi} = p_2 = \text{const.}, \left\{ \begin{aligned} m\ddot{r} + \frac{d\Phi}{dr} &= 0 \\ \Phi &= \frac{p_2^2}{2mr^2} + \chi(r, a_1, a_2) \end{aligned} \right.$$

These equations correspond to a Kepler system in polar coordinates, and  $\chi(r, a_1, a_2, \dots)$  is the potential corresponding to an attractive central force. The second equation of motion means  $mr^2\dot{\phi} = p_2$  that is constant under variation of time. With this result, the two previous equations are clearly equivalent to a following unique one-dimensional equation for the radial coordinate  $r$ , which oscillates between two fixed values. In effect, as it is easily seen, this last expression (see slide S11/1) is analogous to that one

describing the one-dimensional oscillator, and because of that Ehrenfest can apply his adiabatic hypothesis to this motion in the same way he had in the previous example.

Having taken account of the fact that  $p_2$  is also invariant under variations of the parameters  $a_1, a_2 \dots$ , Ehrenfest obtains a second quantization rule (see slide S11/2). On the other hand, by applying independently the Sommerfeld quantization rules to the Kepler system in polar coordinates, the quantization has exactly this form for each one of the coordinates:

HQI-S11/2

By the Ehrenfest's adiabatic hypothesis:

$$\frac{\overline{2T_1}}{\nu_1} = \iint dq_1 dp_1 = ad. inv.$$


$$\frac{\overline{2T_2}}{\nu_2} = \iint dq_2 dp_2 = ad. inv.$$

$q_1$  is the radial variable  
and  $q_2$  the angular variable

↔

Sommerfeld quantization:

$$\iint dq_1 dp_1 = 0, h, \dots, nh, \dots$$

$$\iint dq_2 dp_2 = 0, h, \dots, nh, \dots$$


This procedure is valid for all central forces

Hence, both ways to quantize are, in this case, equivalent. Ehrenfest also states this procedure to be valid for all central forces, since any central force can be connected to the Kepler system adiabatically by changing infinitively slowly the corresponding parameters on which the central potential depends.

Up to this point, Ehrenfest has proved the compatibility of his hypothesis with all different quantization rules that had appeared until that moment. The only quantization rule that Ehrenfest does not mention is Bohr's one, probably because he thought of it unfavourably by then.

### Difficulties: Singular Motions

However, in applying the hypothesis some difficulties appear. By analyzing the adiabatic transformation of the movement of an electric dipole from a vibration to a rotation by diminishing the orienting field  $\vec{E}$ , it is possible to better understand these difficulties (see slide S<sub>12</sub>). In path 1, just in the transition movement between vibration and rotation, a motion with an infinite period emerges, in which it is impossible to define an infinitively slow change, that is, an adiabatic transformation, as the change rate is always defined in reference to the period of motion. Then, Ehrenfest's adiabatic hypothesis cannot be applied at this point. As a visible consequence of this fatal ambiguity, after this motion, the electric dipole can rotate clockwise or counter clockwise.

Ehrenfest proposes an alternative transformation to shun this problem (see *path 2*). In this picture, the dipole does not oscillate in a single plane, but it does so conically, so that after varying the value of the electric field adiabatically, from a finite number

## The Ehrenfest Adiabatic Hypothesis and the Old Quantum Theory

to zero, the final motion has no indetermination and the electric dipole has not passed through a singular motion.

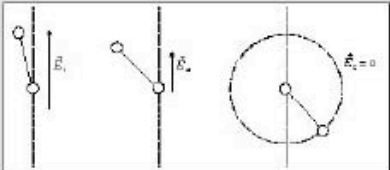
This second path avoids the ambiguity, but does not get rid of this dark point in the whole coherence of the Ehrenfest adiabatic hypothesis. In principle, it would be necessary to justify the plausibility of *path 1*. Ehrenfest hints that solving this question could be related to a possible extension of the application of his hypothesis to aperiodic motions.

HQ1-S12

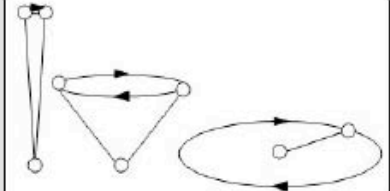
### Difficulties: singular motions

**Electric dipole**

*Path 1:* Indetermination in the final motion, as the dipole passes through a singular motion during the adiabatic transformation.



*Path 2:* No indetermination in the final motion, as the dipole doesn't pass through a singular motion during the adiabatic transformation.



### Connection to the Statistical Basis of the Second Law

As we have commented above, in the paper of 1914, Ehrenfest wondered about the compatibility between the quantum theory and the statistical interpretation of the second law of thermodynamics, as the suppositions from which Boltzmann's and Planck's statistics were constructed were quite different. In the first case, all initial conditions—compatible with the corresponding constraints—are possible. On the contrary, in Planck's statistics, not all initial conditions—compatible with constraints—are possible, but only those represented by Planck's ellipses on the phase plane. In the case of Boltzmann's statistics, all regions with equal area on the phase plane are equally probable, while in the case of Planck's statistics, where not all movements are possible, allowed motions are equally likely.


After some calculations and considerations, Ehrenfest deduced in 1914, and exposed again in this 1916 paper, that the validity of Boltzmann's principle is ensured for systems with one degree of freedom if the quantization is applied to adiabatic invariants. This is not the case for systems with more than one degree of freedom, for which this validity—and henceforth its compatibility with the adiabatic hypothesis—still remains doubtful.



HQ1-S13

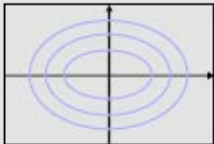
## Connection to the statistical basis of the second law of thermodynamics

**Boltzmann statistics**



- All initial conditions compatible with constraints are possible.
- Regions with equal area in the phase-space are equally probable.

**Planck statistics**



- Not all initial conditions compatible with constraints are possible.
- Possible motions are equally probable.

Does the Boltzmann principle remain valid in the quantum theory?  $\zeta S = k \log W$  ?

- One degree of freedom: if  $\frac{2T}{v} = \iint dqdp$  fixed values.
- More than one degree of freedom: it's still doubtful.

## First Reactions (1916–1918)

In the first half of 1916 new developments of the Sommerfeld theory, which tried to give a solution to the dependence of the quantization on the coordinate system, were published. We are referring to the contributions by Epstein and Schwarzschild, who used the Hamilton-Jacobi theory to try and elucidate for which coordinate system Sommerfeld rules could be applied. These contributions dealt with multiperiodic motions, which are, in a sense, made up by partial periodic motions for each of its coordinates.

This kind of motions can be defined accurately through the Hamilton-Jacobi equation:

$$H\left(q_1, \dots, q_n; \frac{\partial S}{\partial q_1}, \dots, \frac{\partial S}{\partial q_n}\right) + \frac{\partial S}{\partial t} = 0$$

( $S$  is the generatrix function of a transformation that converts the original coordinates  $q_1 \dots q_n$  into constants of motion). In the case of separable systems (systems where the Hamilton-Jacobi equation is separable), it is possible to obtain, in some coordinate systems, one Hamilton-Jacobi equation for each coordinate. That is:

$$H_i\left(q_i; \frac{\partial S}{\partial q_i}; \alpha_1, \dots, \alpha_n\right) + \frac{\partial S_i}{\partial t} = 0$$

( $S_i$  only depends on the coordinate  $q_i$ , on  $n$  different constants of motion  $\alpha_1 \dots \alpha_n$ , and on time  $t$ ). In other words, in separable systems the generatrix function  $S$  has the form:

$$S = \sum_i S_i(q_i; \alpha_1, \dots, \alpha_n; t).$$

Epstein and Schwarzschild stated that only in such cases was it possible to apply the quantization to the different phase integrals without ambiguities: the correct quantization was that one obtained in the coordinate system where the Hamilton-Jacobi equation was separable.

HQ1-S14

## Multiperiodic systems

- $\iint dq_i dp_i = 0, h, \dots, n_i h, \dots \Leftrightarrow$  in certain cases depends on the coordinate system.
- Epstein and Schwarzschild use H-J theory  $H\left(q_1, \dots, q_n; \frac{\partial S}{\partial q_1}, \dots, \frac{\partial S}{\partial q_n}\right) + \frac{\partial S}{\partial t} = 0$

If the system is separable,

$$H_i\left(q_i; \frac{\partial S_i}{\partial q_i}; \alpha_1, \dots, \alpha_n\right) + \frac{\partial S_i}{\partial t} = 0$$

$S = \sum_j S_j(q_j; \alpha_1, \dots, \alpha_n; t)$ , where  
 $\alpha_1, \dots, \alpha_n$  are constants of motion.

➔

$I_i = \oint p_i dq_i = n_i h$

In the coordinate system where the H-J equation is separable, are  $I_i$  adiabatically invariant?

This new contributions reduced the problem to the so called ‘degenerate motions’. This class of motions can be characterized through its ‘proper’ frequencies: frequencies of degenerate motions satisfy one or more ‘commensurability relations’, and frequencies of non degenerate ones does not (see slide  $S_{15}$ ). In the former, the separation of variables can be done in more than one system of coordinates, so that an ambiguity remained in how quantization should be applied.

In the postscript of his 1916 paper, Ehrenfest wondered if the phase integrals referred by Epstein, Schwarzschild, and Sommerfeld were adiabatically invariant. It was for this reason that Ehrenfest entrusted his disciple Burgers with the task of finding an answer to this question.

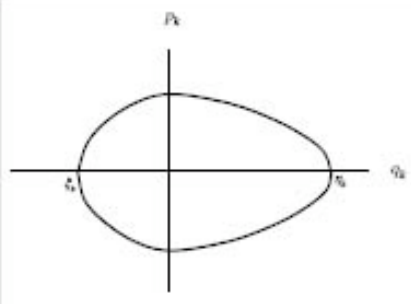
Very soon, in December of the same year and January of the next one, Burgers obtained a definite result. He found that, in the case of non degenerate motions, the phase integrals were always adiabatically invariant, whereas in the case of degenerate motions, only certain linear combinations of these phase integrals were so only if the degree of degeneration (the number of commensurability relations) remained constant during the adiabatic transformation.

HQ1-S15

## Burgers (1916-1917)

Are  $I_k = \oint p_k dq_k$  adiabatically invariant?

In separable systems, there are  $p$  independent periodic motions, with frequencies  $\nu_i$ :



- Non degenerate motions:  $\sum_{i=1}^p m_i \nu_i \neq 0$   
( $m_i$  are whole numbers)  
 $\Rightarrow$  H-J equation is separable only for one coordinate system
- Degenerate motions:  $\sum_{i=1}^p m_i \nu_i = 0$   
 $\Rightarrow$  H-J equation is separable in more than one coordinate system

- In the case of non degenerate motions,  $\delta' I_k = \delta \oint dq_k dp_k = 0$  always.
- In the case of degenerate motions,  $\delta' Y_s = \delta \sum_k r_s^k I_k = 0$  only in certain cases.

This contribution of Burgers must be considered, not as a new application of the Ehrenfest's hypothesis, but as a part of it, as it perfectly completed the exposition contained in the 1916 paper and contributed to improve its theoretical basis, extending the proof of the compatibility of the adiabatic hypothesis with the quantum rules which appeared after Ehrenfest had redacted his work.

Apart from Burgers, two former disciples of Ehrenfest, Kramers and Krutkow, also contributed to give foundation to the adiabatic hypothesis in similar ways. Kramers, who had been installed in the summer of 1916 in Copenhagen as Bohr's collaborator, tried to go further than Burgers, and began writing a manuscript where he was to study the adiabatic transformations in degenerate systems more deeply. In this manuscript, Kramers assesses that Burgers' proof could be generalized to relativistic systems. As far as we know, this manuscript was never published, but Kramers sent a copy to Ehrenfest in the summer of 1917.

HQ1-S16

## Contributions to the adiabatic hypothesis, before Bohr

- **Burgers** (1916-1917; "Adiabatic invariants of mechanical systems. I, II, III". *Proceedings of the Amsterdam Academy* 20, 149-157, 158-162, 163-169): He proves the adiabatic invariance of phase integrals for non degenerate multi-periodic motions.
- **Kramers** (1917; "On the adiabatic invariants of mechanical systems". *Unpublished manuscript*): He studies the degenerate motions more deeply and he considers also the relativistic case.
- **Krutkow** (1919; "Contributions to the theory of adiabatic invariants". *Proceedings of the Amsterdam Academy* 21, 1112-1123): He proposes a way to find adiabatic invariants.

Krutkow, a friend of Ehrenfest's from his Russian days, who still resided in Saint Petersburg, was only partially aware of Burger's works. He did not know the contribution of 1918 by Bohr either. In late 1918 he sent a paper to Ehrenfest that scarcely contained any novelties, for in it Krutkow only proposed a new way to find adiabatic invariants (the action-angle variables introduced in the quantum theory by Schwarzschild—to which we will not refer here—had solved this particular question; moreover Burgers had proved in the third paper of his contribution to the Amsterdam Academy the compatibility between the Schwarzschild approach and the adiabatic hypothesis). Anyway, Ehrenfest decided to publish it in the *Proceedings of the Amsterdam Academy*.

But all of these contributions did not contain any new applications of the adiabatic hypothesis. They were destined for showing the harmony that existed between Ehrenfest's idea and the quantum theory. As far as we know, in 1917 and 1918, the adiabatic hypothesis was *used* only in five papers: two by Smekal, one by Planck, one by Sommerfeld, and one by Bohr.

Smekal, who was a young physicist when he moved to Berlin to finish his studies, published then, in 1918, two papers in the *Physikalische Zeitschrift* about the adiabatic hypothesis. They were basically centred on its statistical connections. Mainly he tried to generalize the considerations about the validity of Boltzmann's principle to systems with more than one degree of freedom.

Also in 1918, Planck used the hypothesis to choose one of the two possible quantizations found for the asymmetric spinning top (a rigid solid with three different moments of inertia). In this case, Planck privileged the quantization that was in agreement with

the adiabatic hypothesis by Ehrenfest.

HQ1-S17

## Uses of the adiabatic hypothesis (1917-1918)

- Related to statistical implications of the adiabatic hypothesis:
  - Smekal (1918; "Über die zum Beweise des Boltzmannschen Prinzips verwendete „wahrscheinlichste“ Verteilung", "Adiabatenhypothese und Boltzmannschen Prinzip". *Physikalische Zeitschrift* 19, 7-10, 137-142).
- Applications:
  - Planck (1918; "Zur Quantelung des asymmetrischen Kreisel". *Preussische Akademie der Wissenschaften*, 1166-1174). Quantization of the asymmetric spinning top.
  - Sommerfeld (1917; "Die Drudesche Dispersionstheorie vom Standpunkte des Bohrschen Modelles und die Konstitution von  $H_2$ ,  $O_2$  und  $N_2$ ". *Annalen der Physik* 53, 497-550). On light's dispersion.

Sommerfeld used Ehrenfest's hypothesis to give a basis to his treatment of the magnetic field influence on the trajectory of the electrons in a paper on light's dispersion. Sommerfeld stated that Ehrenfest's rule, which restricted the quantization only to adiabatic invariants, ensured the validity of the mechanical laws during slow transformations.

As we can see, all these uses are, in a way, minor uses. Because of that, we assess that the first response to Ehrenfest's publication was rather scarce, almost null. On the other hand, as we have seen, the works of Burgers, Kramers and Krutkow can not be considered as new applications or true reactions, because all of them contain attempts to give solid reasons to present the adiabatic hypothesis as a fundamental rule for the quantum theory. Moreover, only the papers by Burgers were often quoted in the following years. But this scenario changed abruptly when Bohr published his new theory.

## The Adiabatic Hypothesis in Bohr's 1918 Paper

The first part of *On the quantum theory of line spectra* was published in April of 1918 as a memory of the Danish Real Academy. Its diffusion was not fast—the war had not finished yet—, but it gradually became one of the essential works of the quantum theory. This part contained the general theoretical basis of Bohr's theory, and the second one—published in December—contained a detailed analysis of the spectrum of the hydrogen

## The Ehrenfest Adiabatic Hypothesis and the Old Quantum Theory

atom. It was with the publication of the first part that a new stage of the role that Ehrenfest's adiabatic hypothesis played in the development of quantum ideas began.

HQI-S18

### The adiabatic hypothesis in Bohr's paper of 1918

ON  
THE QUANTUM THEORY  
OF LINE-SPECTRA  
BY  
N. BOHR

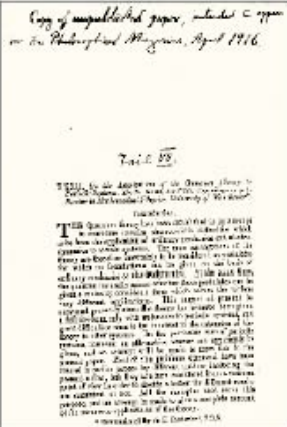
"On the quantum theory of line spectra. Part I".  
*Det Kongelige Danske Videnskabernes Selskab. Matematisk-Fysiske Meddelelser 4(1), 1-36.*

However, this was not the first work where Bohr made use of Ehrenfest results. In early 1916, he had finished a renewed version of his quantum theory of 1913, now extended to all kind of periodic systems. However, when this paper was going to be published in the *Philosophical Magazine*, Bohr received by mail the recent Sommerfeld contributions and decided to restate the whole thing from scratch.

HQI-S19

### Bohr's unpublished theory of 1916

*Copy of unpublished paper, intended to appear in the Philosophical Magazine, April 1916.*



"On the application of the quantum theory to periodic systems"  
*...intended to appear in the Philosophical Magazine, April 1916.*

Bohr uses Ehrenfest's adiabatic invariant to characterize the stationary states:

$$\bar{T} = \oint T dt = \frac{1}{2} nh$$

This paper of 1916 shows that Bohr knew Ehrenfest's work very well, except for the 1914 one about Boltzmann's principle. Two years later, in 1918, he is already a connoisseur of that paper and even uses some of the statistical considerations that appeared in it. In fact, in 1919, he explained to Sommerfeld that it was precisely the lack of a rich statistical approach to the quantum theory that had prevented him from reformulating quickly his results of 1916.

In this theory, Bohr used for the first time the mechanical theorem by Boltzmann-Clausius-Szily rescued by Ehrenfest for the quantum theory, and he proposed to quantize the adiabatic invariant to characterize the stationary states of periodic systems. That is to say, he proposed to generalize Planck's quantum hypothesis the same way as Ehrenfest did. But all of this remained unpublished.

Coming back to Bohr's 1918 work, we must recall that it was based on two postulates. According to the first one, an atomic system could only exist permanently in a specific series of states corresponding to a discontinuous series of values for its energy, which were called 'stationary states'; any transition between two of these states implied a change in the energy of the system. According to the second one, the frequency of the energy emitted or absorbed during such a transition would have the value

$$\nu = \frac{E' - E''}{h}$$

where  $E'$  and  $E''$  are the values of the energy of the two stationary states considered.

In this theory, Bohr included not only the contributions by Sommerfeld, Epstein, and Schwarzschild, but also the transition probabilities introduced by Einstein in 1916 and the principle of the "mechanical transformability", which is the name with which he rebaptized the Ehrenfest's adiabatic hypothesis.

Bohr wanted this principle to function as guarantee of the stability of the stationary states. Thus, according to it, the mechanical laws were valid, not only under constant external conditions, but also during infinitively slow changes of them, that is, during adiabatic transformations:

HQ1-S20/1

## Principle of the "mechanical transformability" (1918)

•Stability of orbits:

*... the motion of an atomic system in the stationary states can be calculated by direct application of ordinary mechanics, not only under constant external conditions, but in general also during a slow and uniform variation of these conditions ...*

## The Ehrenfest Adiabatic Hypothesis and the Old Quantum Theory

This implied that no small change of the motion could provoke quantum jumps, and that by them no emission or absorption processes could take place.

But the adiabatic hypothesis still had another crucial role:

HQ1-S20/2

**• A priori probabilities:**

*If the a-priori probabilities are known for the states of a given atomic system, however, they may be deduced for any other system which can be formed from this by a continuous transformation without passing through one of the singular systems referred below.*

(A “continuous transformation” means an “adiabatic transformation”, and “the singular systems” are related to “the singular motions” to which we have referred above). This passage of Bohr’s paper can be summarized as follows: during an adiabatic transformation, the a priori probabilities for the states remain constant. This assumption about the a priori probabilities of the stationary states links directly to the considerations that Ehrenfest introduced in 1914 and afterwards in 1916 about the validity of Boltzmann’s principle. But while Ehrenfest limited the assessment of the validity of the statistical interpretation of the second law to systems with one degree of freedom, Bohr extends directly this validity to systems with more than one degree of freedom. We must remind that Bohr deals only with stationary states (quantum states) while Ehrenfest does not so.

Apart from these applications, Bohr contributed to extend the implications of the Ehrenfest’s adiabatic hypothesis to more circumstances. For instance, he extended it to relativistic systems, he took profit of the characteristic situation of the degenerate motions to connect different stationary states of the same system, and he also conceived a way to calculate the a priori probabilities in a degenerate system.

HQ1-S21

### Bohr’s contribution to the adiabatic hypothesis

- Boltzmann principle is valid in systems of more than one degree of freedom.
- Extension to the relativistic case.
- Transformations between stationary states of the same system.
- Calculation of a-priori probabilities in degenerate systems.



## Final Remarks

1. As we have shown, the Ehrenfest's adiabatic hypothesis had no considerable impact in the development of the quantum theory before the publication of Bohr's paper of 1918.
2. Despite his own developments, Bohr's use of the adiabatic hypothesis is very close to the original formulation. Because of that, Bohr's principle of mechanical transformability can be considered the most complete version of it.
3. Since 1918, the references to the adiabatic hypothesis increase. They emerged in so different fields as atomic models, specific heats of solids or quantization of aperiodic motions.
4. And, finally, we would like to conclude this talk pointing out that after his paper of 1916, Ehrenfest hardly worked anymore on the adiabatic hypothesis. The only subsequent publication that was related to it was a retrospective paper that the editors of *Die Naturwissenschaften* asked to him to include it in the number of 1923 devoted to celebrate the tenth anniversary of Bohr's atomic model.

## References

- DARRIGOL, O. (1992): *From c-numbers to q-numbers: The classical analogy in the history of quantum theory*. Berkeley, University of California Press.
- JAMMER, M. (1966): *The conceptual development of quantum mechanics*. New York, Mc-Graw Hill.
- KLEIN, M. J. (1985): *Paul Ehrenfest. The making of a theoretical physicist*. Amsterdam, North-Holland. First edition of 1970.
- NAVARRO, L. & PÉREZ, E. (2004): "Paul Ehrenfest on the necessity of quanta (1911): Discontinuity, quantization, corpuscularity, and adiabatic invariance". *Archive for History of Exact Sciences* 58, 97–141.
- NAVARRO, L. & PÉREZ, E. (2006): "Paul Ehrenfest: The genesis of the adiabatic hypothesis, 1911–1914". *Archive for History of Exact Sciences* 60, 209–267.

## 6 Re-Examining the Crisis in Quantum Theory, Part 1: Spectroscopy

DAVID C. CASSIDY

One of the topics set for this workshop touches upon the transition from the old quantum theory to the new quantum mechanics—in particular, “how the physics community came to recognize the limitations” of the old quantum theory.<sup>1</sup>

Some of the answers to this question may be found in one of the most unsettled periods in the history of quantum physics. These were the years between the end of the First World War in 1918 and the breakthrough to quantum mechanics in 1925–27. It was a period of great difficulty and upheaval, but also remarkable creativity—both for quantum physics and for European society, Germany in particular.

Paul Forman and others have long recognized the remarkable simultaneity of events occurring at that time in the realms of physics and society. Equally remarkable is the appearance during this period of public expressions of a crisis situation within both realms. For example, while Oswald Spengler prophesied the *Untergang des Abendlandes*, a number of physicists, among them Einstein, lamented what he called “The present crisis of theoretical physics.”<sup>2</sup> In both physics and society those years were indeed, to quote the title of another book by Spengler, *Jahre der Entscheidung*.<sup>3</sup>

What was going on here? What developments inside and outside the old quantum theory could lead a large number of quantum physicists to doubt the possibility of further progress using that theory? In what sense and to what extent could this be regarded as a “crisis” situation? Was there really any connection between the simultaneous events occurring within physics and society?

These are all very profound and far-reaching historical questions. But, of course, they are not new. This year marks not only the 60th anniversary of the passing of Max Planck in 1947, but also the 40th anniversary of the completion of the Archive for History of Quantum Physics and the publication of its catalogue in 1967.<sup>4</sup>

Greatly stimulated in part by the availability of this archive, during the past half century a large number of historical studies have been devoted to answering many of the fundamental questions about this fertile period of transition from the old to the new

---

<sup>1</sup>MPIWG, “Conference on the history of quantum physics, 2–6 July 2007, Berlin.”

<sup>2</sup>Oswald Spengler, *Der Untergang des Abendlandes*, 2 vols. (Munich: C. H. Beck, 1918); Albert Einstein, “Über die gegenwärtige Krise der theoretischen Physik,” *Kaizo* (Tokyo), 4 (1922), 1–8, reprinted, Karl von Meyenn, ed., *Quantenmechanik und Weimarer Republik* (Braunschweig: Vieweg, 1994), 233–239, quote on 238–239. The talk of a crisis was not new in physics. It appeared before the war in, for instance, Paul Ehrenfest, *Zur Krise der Lichtäther-Hypothese* (Berlin: Springer, 1913). I thank Skúli Sigurdsson for bringing this to my attention.

<sup>3</sup>Oswald Spengler, *Jahre der Entscheidung*, erster Teil (Munich: C. H. Beck, 1933).

<sup>4</sup>Thomas S. Kuhn et al., eds., *Sources for history of quantum physics: An inventory and report* (Philadelphia: Am. Philosophical Society, 1967).

quantum physics.

Looking back over the past decades, two important historiographic works regarding the crisis in quantum theory immediately spring to mind.

## Historiographic Works

1. Thomas S. Kuhn, *The Structure of Scientific Revolutions*, 1962.

For Kuhn, crises entail a rupture between two paradigms, caused mainly by internal developments within normal science. Kuhn described a crisis situation this way:

“Because it leads to large-scale paradigm destruction . . . the emergence of new theories is generally preceded by a period of pronounced professional insecurity. As one might expect, that insecurity is generated by the persistent failure of the puzzles of normal science to come out as they should.”<sup>5</sup>

2. Paul Forman, “Weimar Culture, Causality, and Quantum Theory, 1918–1927,” 1972, takes Kuhn one step further regarding the crisis in quantum theory:

“While it is undoubtedly true that the internal developments in atomic physics were important in precipitating this widespread sense of crisis . . . nonetheless it now seems evident to me that these internal developments were not in themselves sufficient conditions. The *possibility* of the crisis of the old quantum theory was, I think, dependent upon the physicists’ own craving for crises, arising from participation in, and adaptation to, the Weimar intellectual milieu.”<sup>6</sup>

Not until very recently has another work appeared offering a different perspective on the crisis situation in quantum theory.

3. Suman Seth, “Crisis and the construction of modern theoretical physics,” March 2007.

According to Seth, “Different subgroups within theoretical physics viewed the situation in dramatically different ways,” depending upon their differing research agendas.

- “Members of the Sommerfeld school in Munich, who saw the task of the physicist as lying in the solution of particular problems, neither saw a crisis nor acknowledged its resolution.”
- “Researchers associated with Bohr’s institute in Copenhagen, who focused on the creation and adaptation of new principles, openly advocated a crisis even before decisive anomalies arose.”<sup>7</sup>

---

<sup>5</sup>Thomas S. Kuhn, *The Structure of Scientific Revolutions* (Chicago: University of Chicago Press, 1962), pp. 67–68.

<sup>6</sup>Paul Forman, “Weimar Culture, Causality, and Quantum Theory, 1918–1927: Adaptation by German Physicists and Mathematicians to a Hostile Intellectual Environment,” *Historical Studies in the Physical Sciences*, 3 (1972), 1–115, on 62; German translation in: von Meyenn, note 2, 61–179.

<sup>7</sup>Suman Seth, “Crisis and the construction of modern theoretical physics,” *British Journal for History of Science*, 40 (March 2007), 25–51, on p. 25.

## Historical Works

Historical studies of the crisis period over the past forty years display a similar pattern—an initial flurry of work on the origins and evolution of quantum physics, followed by a quantum gap as historians turned to other topics, ending with a revival of interest in recent years. Here are some examples:

- M. Jammer. *The Conceptual Development of Quantum Mechanics*, 1966.
- P. Forman. “The doublet riddle and atomic physics circa 1924,” *Isis*, 59 (1968), 156–174.
- P. Forman. “Alfred Landé and the anomalous Zeeman Effect,” *HSPS*, 2 (1970), 153–261.
- H. Small. *The Helium Atom in the Old Quantum Theory*, PhD diss., 1971.
- R. Stuewer. *The Compton effect: Turning point in physics*, 1971.
- D. Cassidy. *Werner Heisenberg and the Crisis in Quantum Theory, 1920–1925*. PhD diss., 1976.
- D. Serwer. “Unmechanischer Zwang: Pauli, Heisenberg, and the Rejection of the mechanical atom, 1923–1925,” *HSPS*, 8 (1977), 189–256.
- J. Hendry. “Bohr-Kramers-Slater: A virtual theory of virtual oscillators,” *Centaurus*, 25 (1981), 189–221.
- Gap—
- O. Darrigol. *From c-numbers to q-numbers: The classical analogy in the history of quantum theory*, 1992. Chapter 8, “A Crisis”.
- H. Kragh. *Quantum generations: A history of physics in the 20th century*, 1999. Section: “Quantum anomalies”.

In addition to these studies, the last few decades have brought us the publications of the Pauli correspondence, the Born-Einstein letters, the Sommerfeld-Nachlass, and the collected papers of nearly every major physicist of the era, along with many online resources.

With the availability of all of these pioneering works and interpretations, and a rich trove of primary source material, I think we may now be in a position to make the leap to a new quantum state—a re-examination of the quantum crisis at a much deeper level as both history and historiography, thereby achieving a much fuller understanding of what happened and why.

## Origins of the Crisis

Re-examining the mounting problems arising within quantum theory during the early 1920s, we are soon lead back far earlier than 1918, all the way back to the introduction of the quantum itself by Planck and Einstein beginning in 1900, and to the Bohr-Sommerfeld theory of the atom in 1913–16.

While the nature of light and the quantum remained persistent problems, it was the Bohr atom of 1913 and its extensions by Sommerfeld that lay at the foundation of the later crisis situation in quantum atomic physics. It was a critical situation that reached an apex ironically with the celebration of the 10th anniversary of the Bohr atom in 1923. I would like to point out briefly several implications of this theory.

## The Bohr Atom

- It provided an extraordinarily successful visualizable mechanical model of orbiting electrons in stationary states obeying classical mechanics but not electrodynamics. It accounted for stability, optical spectra, and ionization of hydrogen atoms.
- Despite this success, many statements appeared over the next decade on the fundamentally unsatisfactory nature of the theory, starting with Bohr himself in 1913. For instance, James Jeans declared: “The only justification at present put forward for these assumptions is the very weighty one of success . . . It would be futile to deny that there are difficulties, still unsurmounted, which appear to be enormous.”<sup>8</sup>
- Yet the success of the Bohr atom (with extensions by Sommerfeld) set the standard for over a decade of a successful quantum theory of atomic phenomena.
- It became the definition, if you will, of normal quantum atomic science. In this science, what was frequently called “eine modellmäßige Deutung,”—“a modelbased interpretation/ explanation”—of atomic phenomena became the goal of a successful theory, what Heisenberg and Pauli later called a “physical explanation.”

## My Points

With the Bohr atom as a background, my argument regarding the crisis in quantum theory is composed of the following points:

- Beginning about 1918, new and more precise data and mechanical calculations resulted by the early 1920s in an increasing failure to achieve the ideal set by the Bohr atom. At the same time, new funding strategies during the post-war economic crisis in Germany provided a boost directly to atomic research.
- The failure of the theory magnified the sense of professional insecurity about the old quantum theory within the community of physicists and mathematicians.
- The insecurity reached such proportions by 1923 that it came close to what Kuhn described as a crisis situation. At the same time, as Seth has suggested, noticeable differences did appear among different groups. However,
- The old quantum theory did in fact work quite well for many other phenomena, such as molecular band spectra.<sup>9</sup>
- The Forman thesis and related issues regarding the quantum crisis are addressed in a separate paper.<sup>10</sup>

---

<sup>8</sup>James Jeans, address to British Association, reported in *Nature*, 92 (1913), 304–309; quoted by Ulrich Hoyer, introduction to Niels Bohr, *Collected Works*, vol. 2 (Amsterdam: North-Holland, 1981), 124.

<sup>9</sup>For example, Edwin Kemble, “The application of the correspondence principle to degenerate systems and the relative intensities of band lines,” *Physical Review*, 25 (1925), 1–22.

<sup>10</sup>D. Cassidy, “Heisenberg, Weimar culture, and the Forman thesis,” paper delivered to conference on 35th anniversary of Forman’s paper, Vancouver, March 2007.

### Three Critical Problems, Three Groups, Three Places—Roughly Defined

In my rather internal re-examination of this period, I have identified three main problem areas, involving three main research groups in three different places, that caused increasing trouble.

1. *Problem:* Multiplet (complex) line spectra of atoms and their anomalous Zeeman effects. Research group: Sommerfeld school in Munich, including Tübingen spectroscopists Friedrich Paschen, Ernst Back with theorist Alfred Landé.
2. *Problem:* Simple 3-body atomic/molecular systems beyond hydrogen atom:  $H_2^+$ , normal  $He$ , and excited  $He$ . Research group: Born school in Göttingen, including Pauli and Heisenberg, also Sommerfeld, Kramers, Kemble, and Van Vleck. Both of these problem areas concerned atomic structure. The third problem area involved the nature of light.
3. *Problem:* Interaction of radiation and matter, including dispersion theory and the existence of light quanta. Research group: Bohr school in Copenhagen, including Pauli, Heisenberg, Kramers.

### Sommerfeld and the Anomalous Zeeman Effect

As also discussed recently by Suman Seth and others, but with somewhat different interpretation, the problem of the Zeeman effect arose within quantum atomic theory as early as 1913, when Bohr sent a copy of his first paper on the Bohr atom to Sommerfeld. Sommerfeld replied immediately: “Will you also apply your atomic model to the Zeeman effect? I would like to concern myself with this.”<sup>11</sup>

Sommerfeld did work on the problem, and in 1916 he published his fundamental paper “Zur Quantentheorie der Spektrallinien,” which established the Bohr-Sommerfeld quantum theory of atomic structure.<sup>12</sup> I will list only briefly some of the important elements of this paper for our purposes:

- The Sommerfeld quantum conditions, involving only *integral numbers of quanta*
- a relativistic treatment of the Kepler orbits of the electrons in the Bohr model led to angular momentum as a degree of freedom, and . . .
- two new quantum numbers for the orbital motion of an electron, giving 3 altogether:  $n$  the state number;  $k$  for azimuthal angular momentum;  $m$  for space quantization, if a  $z$ -axis is defined.

Sommerfeld intended to define the  $z$ -axis by a weak magnetic field and thus obtain the Zeeman effect. He did so in a follow-up paper that same year, as did Peter Debye. The

---

<sup>11</sup>Sommerfeld to Bohr, 4 Sept. 1913, in Bohr, note 8, vol. 2, 603.

<sup>12</sup>Sommerfeld, “Zur Theorie der Spektrallinien,” 3 parts, *Annalen der Physik*, 51 (1916), 1–94 and 125–167; reprinted in Arnold Sommerfeld, *Gesammelte Schriften*, vol. 3 (Braunschweig: Friedrich Vieweg & Sohn, 1968), 172–308.

result was the normal Zeeman effect of hydrogen and other singlet line spectra in a weak magnetic field defining the  $z$ -axis.<sup>13</sup>

$$E = E_0 + \frac{mh}{2\pi} \cdot \frac{eH}{2m_e c} = E_0 + mh\nu_L \quad \text{where } \Delta m = \pm 1, 0$$

where  $E$  is the energy of a Zeeman term,  $E_0$  is the energy of the unperturbed optical  $L$  term, and  $\nu_L$  is the Larmor frequency. This gives the splitting of a singlet line into 3 lines in a weak magnetic field, but the origin of the selection rule was unknown, and the theory could not account for the more prevalent anomalous Zeeman effect.

### Anomalous Zeeman Effect

The effect was associated with the puzzling appearance of optical multiplet lines: the splitting of single lines into closely spaced doublets and triplets. The doublet sodium  $D$ -lines are a well known example. (As we know today, they arise from spin-orbit coupling within the atom.) Unlike singlets, which display the normal Zeeman effect, the multiplet lines split into more than 3 lines or into 3 lines that are not separated by the Larmor frequency. Furthermore, Paschen and Back had discovered by 1913 the so-called Paschen-Back effect, whereby the anomalous lines all coalesce continuously into the normal Zeeman triplet as the external magnetic field is increased.<sup>14</sup> In 1919 Sommerfeld listed this behavior and the appearance of the anomalous Zeeman effect among the “Schwebende Fragen der Atomphysik” (unsettled questions of atomic physics). Question number 1 entailed “eine modellmassige Deutung” of these phenomena, for which, he declared, “entirely new things” were required.<sup>15</sup>

### Sommerfeld’s Program

With new and more precise data pouring into his Munich institute from Tübingen, Sommerfeld set out to find the “entirely new things” in a program explained in paper published in 1920. But it entailed an obvious retreat for the author of the relativistic quantum model of the atom. For Sommerfeld the situation seemed similar to that in hydrogen spectroscopy before the Bohr atom. As Balmer had done decades earlier, Sommerfeld undertook analyses of the highly regular Zeeman data in search of empirical relationships and number harmonies that he hoped would provide clues to the underlying model interpretation of the data. As Seth has argued, Sommerfeld was solving problems not seeking new principles, but, like Balmer, he had little choice at this point.<sup>16</sup>

Sommerfeld soon found what he was looking for. In 1920 he published his famous *Zahlenmysterium*, number mystery. It consisted of a table of number harmonies in

<sup>13</sup>A. Sommerfeld, “Zur Theorie des Zeeman-Effekts der Wasserstofflinien, mit einem Anhang über den Stark-Effekt,” *Physikalische Zeitschrift*, 17 (1916), 491–507; reprinted Sommerfeld, note 12, 309–325; Peter Debye, “Quantenhypothese und Zeeman Effekte,” *Phys. Zs.*, 17 (1916), 507–512.

<sup>14</sup>F. Paschen and E. Back, “Normale und anomale Zeeman effekte,” *Annalen der Physik*, 39 (1912), 897–932. For the phenomena of the Zeeman effect as observed at that time, see A. Sommerfeld, *Atombau und Spektrallinien* (Braunschweig: F. Vieweg & Sohn), 1st edition 1919, 3rd edition 1922, 4th edition 1924. The effect is also discussed in the literature cited earlier.

<sup>15</sup>A. Sommerfeld, “Schwebende Fragen der Atomphysik,” *Phys. Zs.*, 21 (1920), 619–620; reprinted in Sommerfeld, note 12, vol. 3, 496–497.

<sup>16</sup>A. Sommerfeld, “Ein Zahlenmysterium in der Theorie des Zeeman effktes,” *Naturwiss.*, 8 (1920), 61–64 on 64; reprinted in Sommerfeld, note 12, vol. 3, 511–514.

which he had traced the observed multiplet lines to combinations of quantum states to which he assigned empirical “inner quantum numbers”  $j$ . In his scheme, each angular momentum state  $k$  split into two or three states with values of  $j = k, k - 1$  for doublets,  $j = k, k - 1, k - 2$  for triplets. Thus, for example, the sodium  $D$ -lines arise from downward jumps from  $k = 2, j = 2$  to  $k = 1, j = 1$  ( $D_2$ ) and  $k = 2, j = 1$  to  $k = 1, j = 1$  ( $D_1$ ). Sommerfeld believed the inner quantum numbers referred to some unknown inner rotation and “hidden” mechanical quantum condition.

We must be clear about what Sommerfeld was doing. He was not really engaging in number mysticism. Rather, he was attempting to solve a mystery. He was taking the phenomenological approach because he has no other choice, and he is not happy about it. Wrote Sommerfeld, “The musical beauty of our number table will not hide the fact that it presently represents a number mystery. In fact I do not yet see any way to a model-based explanation either of the doublet-triplet data or of their magnetic influence.”<sup>17</sup>

There is none of the sense of desperation and distress expressed by some others at that time. But it does seem to me that Sommerfeld was already participating in what Kuhn called “a pronounced professional insecurity” about the ultimate success of his program. This became more acute following the work of theorists Landé and Heisenberg during the time they participated as collaborators in the Sommerfeld School.

### Landé’s $g$ -Factors

Alfred Landé managed to take Sommerfeld’s number mystery one step further. Very briefly, he associated each multiplet term,  $j$ , with a series of Zeeman terms, each characterized by the magnetic quantum number  $m$  and an empirical “gyromagnetic” factor  $g$ .<sup>18</sup> But his most controversial innovation was the introduction of half-integer values for the magnetic numbers  $m$  of the doublet states on purely empirical grounds. Half integers were required in order to achieve an even number of magnetic states for each value of  $j$ , as shown below.

Landé, 1921:

$$\begin{array}{ll}
 E = E_0 + mh\nu_L & \text{normal Zeeman effect} \\
 E = E_i + gmh\nu_L & \text{anomalous Zeeman effect}
 \end{array}$$

$$\begin{array}{ll}
 g = 1 & \text{singlets} \\
 g = 2j/(2k - 1) & \text{doublets}
 \end{array}$$

$$g = \left\{ \begin{array}{l} 1 + 1/k \\ 1 - 1/(k + 1)(k - 1) \\ 1 - 1/(k - 1) \end{array} \right\} \begin{array}{l} j = k \\ j = k - 1 \\ j = k - 2 \end{array} \quad \text{triplets}$$

$$\begin{array}{ll}
 m = 0, \pm 1, \pm 2, \dots, \pm j & \text{triplets, } 2j + 1 \text{ states, odd} \\
 m = \pm \frac{1}{2}, \pm \frac{3}{2}, \pm \frac{5}{2}, \dots, \pm (j - \frac{1}{2}) & \text{doublets, } 2j \text{ states, even}
 \end{array}$$

<sup>17</sup>Ibid., 64. The number table contained the so-called Runge fractions for the Zeeman terms.

<sup>18</sup>Alfred Landé, “Über den anomalen Zeemaneffekt (Teil I),” *Zs. f. Physik*, 5 (1921), 231–241. Discussed at length by Forman, “Alfred Landé and the anomalous Zeeman Effect,” *HSPS*, 2 (1970), 153–261.



Sommerfeld was ecstatic: “Bravo, you are able to work miracles!” he wrote Landé. “Your construction of the doublet Zeeman types is very beautiful.”<sup>19</sup> To Einstein he wrote, “Light, or better, dawn really is coming to spectroscopy.”<sup>20</sup>

But Sommerfeld and Landé also acknowledged the lack of a model interpretation of the empirical  $g$ -factors along with their continuing hope for a satisfactory model. A model interpretation did soon appear, but it made matters only worse. It showed that the  $g$ -factors and all of the empirical number harmonies could be reduced to a model only if the model was so radical as to force an explicit break with the Bohr-Sommerfeld ideal—in particular a violation of space quantization in a field, and the introduction of actual half-integer angular momenta.

The model was Heisenberg’s Rumpf or core model of the atom, submitted in 1921 as his first published paper while still only a 3 semester student.

## Heisenberg’s Core Model

Heisenberg’s core model arose directly from Sommerfeld’s latest insight: a derivation of Landé’s  $g$ -factors from a “quantum-theoretical reinterpretation” of a classical harmonic oscillator model of the atom proposed earlier by Woldemar Voigt. In December 1921 Sommerfeld submitted a paper titled: “Quantentheoretische *Umdeutung* der Voigtschen Theorie des anomalen Zeemaneffektes vom  $D$ -Linientypus.”<sup>21</sup> I believe the title and the approach of this paper had a direct influence on Heisenberg’s *Umdeutung* paper four years later. Heisenberg’s core model paper was submitted 7 days after Sommerfeld’s *Umdeutung* and published immediately following it in *Zeitschrift für Physik*.<sup>22</sup>

In his paper, Sommerfeld had obtained an equation for the energy of a Zeeman term for doublet lines as a function of the external magnetic field. The equation, shown in the slide below, yields Landé’s doublet  $g$ -factors for small magnetic field, and it displays the Paschen-Back effect for the continuous transition to the normal Zeeman effect as magnetic field increases. (Today, this equation appears as the off-diagonal matrix elements for the energy operator in quantum mechanics.)

The Sommerfeld-Voigt equation for doublets (1921) reads

$$E = E + h\nu_L \left( m^* \pm \frac{1}{2} \sqrt{1 + (2m^*/k^*)\gamma + \gamma^2} \right) ,$$

where  $E$  is the energy of the Zeeman term,  $E$  the average of the doublet energies and

$$\gamma = \frac{\Delta\nu}{\nu_L} \propto \frac{1}{H} \quad , \quad k^* = k - \frac{1}{2} \quad , \quad j^* = j - \frac{1}{2}$$

$$m = \pm \frac{1}{2}, \pm \frac{3}{2}, \dots, \pm -k^* \quad , \quad |m^*| \leq j^* .$$

<sup>19</sup>Sommerfeld to Landé, 25 Feb. 1921, published in Forman, note 18, p. 249.

<sup>20</sup>Sommerfeld to Einstein, 17 Oct. 1921, published in Einstein and Sommerfeld, Briefwechsel, ed. Armin Hermann (Basel: Schwabe, 1968), p. 94.

<sup>21</sup>Sommerfeld, *Zs. f. Physik*, 8 (1922), 257–272; reprinted in Sommerfeld, note 12, vol. 3, 609–624.

<sup>22</sup>W. Heisenberg, “Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen,” *Zs. f. Physik*, 33 (1925), 879–893; idem, “Zur Quantentheorie der Linienstruktur und der anomalen Zeemaneffekte,” *Zs. f. Physik*, 8 (1922), 273–297.

Heisenberg managed to derive this equation for  $E$  from his core model, and to obtain the triplet  $g$ -factors as well. The following concerns only the doublet factors.<sup>23</sup>

1. Heisenberg noted that doublet atoms are single-valence, while triplet atoms are double valence. A single valence atom, such as sodium, contains a nobel-gas “core” of filled electron shells, with one valence electron in the outer shell.
2. The basic idea of Heisenberg’s model is that the half-integer numbers arise from actual half-integer angular momenta. They are  $\frac{1}{2}$  integral because the valence electron for some reason shares  $\frac{1}{2}$  unit of angular momentum with the core, leaving the valence electron with  $k - \frac{1}{2}$  units of momentum.
3. This reproduces what we now recognize as spin-orbit coupling. The valence electron sets up an internal magnetic field at the site of the core. The doublet term structure arises from the parallel or anti-parallel alignment of the core, resulting in a total angular momentum of  $j$  units, where

$$\begin{aligned} j &= \left(k - \frac{1}{2}\right) + \frac{1}{2} = k \quad , \\ j &= \left(k - \frac{1}{2}\right) - \frac{1}{2} = k - 1 \quad . \end{aligned}$$

4. When an external magnetic field is applied, the motion of the valence electron is space quantized, but the core is NOT. It simply aligns itself along the total field vector, changing direction continuously as the external field varies. This results in Sommerfeld’s square-root factor with its continuous transition from the anomalous to the normal Zeeman effect.

Despite Landé’s repeated objections in letters to Heisenberg at that time, Heisenberg held to these and other violations of quantum and classical principles, mainly because the model worked. When Pauli objected, too, Heisenberg responded with his now famous Machiavellian motto: “Der Erfolg heiligt die Mittel.”—“Success sanctifies the means.”<sup>24</sup>

## The Response

And success it was, but at what a cost! Bohr, expressing his own agenda at that time, rejected the model for its violation of integral quantization of angular momenta. His newly successful building-up principle (*Aufbauprinzip*) of the periodic table required integers. Bohr complained to Landé in May 1922:

“My viewpoint is this: that the entire manner of quantization (half integer quantum numbers etc.) does not appear reconcilable with the basic principles of the quantum theory, especially not in the form in which these principles are used in my work on atomic structure.”<sup>25</sup>

---

<sup>23</sup>Further discussed in D. Cassidy, “Heisenberg’s first core model of the atom: The formation of a professional style,” *HSPS*, 10 (1979), 187–224; and Olivier Darrigol, *From c-numbers to q-numbers: The classical analogy in the history of quantum theory* (Berkeley: Univ. California Press, 1992), chapt. 8.

<sup>24</sup>Heisenberg letters to Landé (AHQP Mf 6, 2); Heisenberg to Pauli, 19 Nov. (1921), published in W. Pauli, *Wissenschaftlicher Briefwechsel*, ed. A. Hermann, K. v. Meyenn, V. F. Weisskopf, vol. 1 (Berlin: Springer, 1979), p. 44.

<sup>25</sup>Bohr to Landé, 15 May 1922 (Bohr Scientific Correspondence, Mf 4, 2).

Sommerfeld, on the other hand, once again expressed amazement and delight (and thus approved publication), but he was also perplexed. He wrote to Einstein on 11 January 1922, a now famous statement:

“I have in the meantime uncovered wonderful numerical laws for line combinations in connection with the Paschen measurements and presented them in the third edition of my book. A pupil of mine (Heisenberg, 3rd semester!) has even explained these laws and those of the anomalous Zeeman effect with a model (*Z. f. Ph.*, in press). Everything works out but yet in the deepest sense remains unclear. I can pursue only the technique of the quanta, you must make your philosophy... Set yourself to it!”<sup>26</sup>

This was a remarkable statement for the co-author of the Bohr-Sommerfeld quantum atomic theory. As with the Bohr atom earlier, not only is he fully aware that something is wrong with quantum atomic theory “in the deepest sense,” but also he has now given up the search for a model interpretation as too difficult and is pursuing instead the engineering of empirical data. Pauli and Heisenberg began referring to Sommerfeld’s approach as one seeking formal connections as opposed to physical clarification.

## The Bohr-Festspiel

The unsettled situation in the old quantum theory by 1922 became more unsettled following one of the most important events of the period in quantum theory—Bohr’s series of lectures on atomic structure in Göttingen in June 1922, known as the Bohr-Festspiel.

The hostilities of the world war did not cease with the Armistice in 1918. Because many German scientists had openly supported the German cause during the war, French and British scientists attempted a boycott of German science after the war. While Einstein and Curie worked through the League of Nations to end the boycott, Bohr openly defied it by traveling to Germany on several occasions and inviting German scientists to Copenhagen. In 1922 he accepted an invitation to deliver the Wolfskehl Lectures in Göttingen. The Bohr festival became a turning point. It set the standard for success in quantum atomic theory and thereby rendered the failure to achieve that standard all the more obvious and unsettling.

Over a period of ten days in June 1922, Bohr presented seven lectures on “Die Theorie des Atombaus.”<sup>27</sup> In these lectures he systematically developed what we now view as the old quantum theory of atomic structure. The audience consisted of nearly every major and minor German quantum theorist. Bohr’s systematic approach in his lectures was so impressive that it immediately reenforced at least two research efforts that fall. The first of these, undertaken by Born and Heisenberg in Göttingen, entailed the second problem-area noted earlier: a rigorous and systematic application of celestial mechanics to quantum models of highly excited helium atoms. With the inner electron shielding the +2 charge of the nucleus, the outer electron should give the spectral lines and ionization potential of a perturbed hydrogen atom. The goal was to determine if, under rigorous mechanical calculation, the quantum atomic theory did or did not yield the observed

---

<sup>26</sup>Sommerfeld to Einstein, 11 Jan. 1922, in Einstein and Sommerfeld, note 20, 96–97.

<sup>27</sup>Bohr, “Sieben Vorträge über die Theorie des Atombaus,” 12–22 June 1922 (Bohr Manuscripts, MF 10); published in Bohr, note 8, vol. 4, 341–419.

results. In the end it did not, but I will leave that for another occasion.<sup>28</sup>

The second research program to arise from the Bohr-Festspiel was undertaken by Bohr and Pauli in Copenhagen. Bohr explained it to Landé in March 1923: “It was ... a desperate attempt to remain true to the integer quantum numbers, in which we hoped to see even in the paradoxes a hint for the way in which we might seek the solution of the anomalous Zeeman effect.”<sup>29</sup> The attempt also proved to be a complete failure, and they never published the work. Faced with the inconsistent use of half integers by other theorists, Pauli had had enough. He complained to Bohr in February 1924 that physicists in Germany were using integer and half-integer quantum numbers as they pleased, depending on whether or not they could get the result to agree with experiment. “I myself have no taste for this kind of theoretical physics and retire from it to my heat conduction in solid bodies.”<sup>30</sup>

In light of both of these failures, Max Born summed up the desperate situation for the public in his now famous statement in celebration of the 10th anniversary of the Bohr atom in a special issue of *Die Naturwissenschaften*, published in Bohr’s honor (probably in gratitude for his support of German science) in July 1923: “It is becoming ever more probable that not only new assumptions in the usual sense of physical hypotheses will be necessary, but rather that the entire system of concepts of physics must be rebuilt from the ground out.”<sup>31</sup>

Born and Heisenberg began the search for what Born was now calling a new “quantum mechanics.”

## Conclusion

Even though I have not yet discussed the other two problem-areas to any extent, it is already clear that by mid-1923 the crisis in quantum theory was in full swing. As Seth has suggested, different people and their collaborators reacted to the situation in different ways. While Pauli resigned, Sommerfeld and Landé continued analyzing the data for numerical harmonies, Bohr maintained his consistency, and Born and Heisenberg began the search for a new quantum mechanics. Whatever their response, all appeared to be experiencing, in Kuhn’s words, a “pronounced professional insecurity ... generated by the persistent failure of the puzzles of normal science to come out as they should”—in other words, a crisis in quantum theory.

---

<sup>28</sup>The failure is discussed in several of the works cited earlier in the text, especially those by Small, Darrigol, and Cassidy.

<sup>29</sup>Bohr to Landé, 3 March 1923 (AHQP Mf 4, 1).

<sup>30</sup>Pauli to Bohr, 21 Feb. 1924; published in Pauli, note 24, 147–148.

<sup>31</sup>M. Born, “Quantentheorie und Störungsrechnung,” *Naturwiss.*, 11 (6 July 1923), Heft 27: “Die ersten zehn Jahre der Theorie von Niels Bohr über den Bau der Atome,” pp. 537–542, on 542. See also, A. Landé, “Das Versagen der Mechanik in der Quantentheorie,” *Naturwiss.*, 11 (24 Aug 1923), 725–726, letter dated 15 July 1923.



# 7 The Causality Debates of the Interwar Years and their Preconditions: Revisiting the Forman Thesis from a Broader Perspective

MICHAEL STÖLTZNER

In this paper I have to be sketchy and up-front. Sketchy because I will try to convey the punch line of my 400 page Ph.D.-dissertation (Stöltzner 2005) and the papers ensuing therefrom (Stöltzner 1999, 2000, 2003). I showed there, I guess, that the oft-debated causality debates in Weimar Germany and interwar Austria were an integral part of a much longer causality debate that emerged from two different readings of Boltzmann's legacy, statistical mechanics, at the end of the 19<sup>th</sup> century and ended only in the late 1930s when the philosophical debates surrounding quantum mechanics abated. Viewed within the context of this longer debate, the years 1918–1927 were, no doubt, a time of turmoil ranging from culture and politics to philosophical terminology. But in contrast to Forman (1971), I think, that most scientists seriously pondering about and writing on causality had taken their general philosophical stand already long before. Rather than an adaptation to a hostile intellectual milieu that, in 1927, proved to be of selective advantage, we find a complex but continuous debate about the philosophical consequences of modern physics that, after 1913, mainly appears on the pages of the leading scientific journal of the German-speaking world, Arnold Berliner's *Die Naturwissenschaften*.

Let me be up-front, as was Forman himself when he spoke of his protagonists as “converts to acausality” who made “quasi-religious confessions to the [anti-scientific] milieu”, advocated “existentialism disguised as logical empiricism” (on Reichenbach) and published a book that contained “largely blather” (on Frank 1932). To my mind, Forman's thesis misses core aspects of the causality debate from 1918 to 1927, and it does so because its author followed a methodology that, albeit fruitful in many other domains, is unable to assess the interactions between philosophical and scientific commitments in a historical context of the kind of Weimar Germany and interwar Austria. More generally, in order to appraise the historical dynamics of a philosophical concept, such as causality, any broader historical and sociological approach must be accorded with the recently sharpened methods of the history of philosophy of science.

My own picture of the causality debate is a complex one and it involves philosophical as well as historical, ideological, and sociological motives. Philosophically, the debate about causality and determinism was hardly separable from the quest for a proper interpretation of physical probability, the conception of microphysical reality, and the more general debates about the effects of modern physics on the conception of nature. Some of these lines reached back into the 1890s, when the old mechanical world-view broke into

pieces, and they concerned statistical mechanics, relativity theory, and quantum physics alike. Many critics, among them John Hendry (1980), have noted that Forman's main philosophical misconception was to adopt, as did Spengler, a conception of causality that was intimately linked to the strict determinism that predated statistical mechanics. Already in 1872, Emil du Bois-Reymond had touted the idea that firmly sticking to this explanatory ideal forced scientist to forgo forever a full understanding of the essence of matter and force. Interestingly, in the Weimar days hardly any scientist rehearsed the old *Ignorabimus*, but many considered it the basic misconception responsible for the diagnosis of crisis in modern physics. It is true, Ludwig Boltzmann, in his battles with energeticism, conceived himself as the last exponent of the mechanical world-view. But on the other hand, in developing step-by-step the statistical interpretation of the second law of thermodynamics he introduced a notion that was entirely alien to the mechanical picture which DuBois-Reymond had built upon, to wit, an objective physical probability that could no longer be understood as degree of ignorance.

The debate as to whether physical science at all required a causal foundation started with Franz Serafin Exner's rectorial address of 1908, by which he launched a local tradition of empiricist indeterminism that I call Vienna Indeterminism. Among its main advocates, I count, besides Exner, his former assistant Erwin Schrödinger and the Logical Empiricists Philipp Frank and Richard von Mises. Exner (1909) argued that chance is the basis of all natural laws and that the apparent determinism in the macroscopic domain emerged only as the thermodynamic limit of many many random events. Max Planck, in another rectorial address of 1914 that equally sung the praise of Boltzmann, fiercely objected to Exner's indeterminism and insisted on a deterministic foundation of all natural laws including the probabilistic ones. The debate, as I conceive it, ended on the 1936 Copenhagen Congress for the Unity of Science when Frank and Moritz Schlick, Planck's former student and a resolute critic of any indeterminacy in principle, joined arms to combat the increasing number of metaphysical misinterpretations of quantum mechanics.

My main sociological point is that in the German-speaking world the causality debates were conducted by 'physicist-philosophers', a role model that was more widespread there than in other countries. It had influential historical prototypes, among them Hermann von Helmholtz and Ernst Mach, and there was a clear conduit how a physicist laid claim to it. Most importantly, these philosophical ambitions were only loosely embedded into the then current philosophical schools, among them neo-Kantianism and *Existenzphilosophie*.

Since the philosophical convictions of physicist-philosophers were not forced into a coherent philosophical system, there was ample leeway to simultaneously participate in different thought collectives. This conception that we owe to Ludwik Fleck (1929) is an important clue to understand the seven years the Forman thesis is about. Yes, there were those who defended scientific modernism and technological progress, but diagnosed a cultural crisis. Richard von Mises, for one, still in the 1950s heeded sympathies for Spenglerian ideas. And there were others, like his fellow physicist-philosophers from the Vienna Circle, who at the 1929 Congress of the German Physical Society went public with the claim that the achievements of modern science demanded an entirely new style of scientific philosophizing and, more broadly, a scientific world conception. No wonder that Richard von Mises disliked the manifesto, but he and Frank, in the opening session

of the same congress, appeared almost as intellectual twins in their plea for abandoning the old triad of “school philosophy”, the categories of space, time, and causality, and replacing it with more suitable notions. (Frank 1919, von Mises 1930) This message was well understood by those who rejected the neo-positivist assault on metaphysics, among them the third speaker of the Prague session, physicist-philosopher Arnold Sommerfeld (1929).

My paper is organized as follows. First, I provide a sketch of the causality debate. Second, I characterize the role model of physicist-philosopher and to what extent *Die Naturwissenschaften* provided a forum for this discourse. Third, I historically contextualize the Forman thesis itself and indicate in what way new methodological insights in the history of philosophy of science may prove helpful in understanding the causality debate.

### Vienna Indeterminism and the Causality Debate

Rather than representing merely a “subterranean anticausality current” (Forman 1971, 67), as Forman put it, Exner’s inaugural speech of 1908 made a great stir and triggered a polemic with Planck that continued the earlier Mach-Planck controversy. Frank’s recollections in the interview with T. S. Kuhn show how influential this speech was for the then younger generation of Vienna physicists. Not that Exner in 1908 would have continued Mach’s skepticism about atoms and the energeticist interpretation of thermodynamics. To the contrary, he closely followed the brand of empiricism that Boltzmann had developed from the late 1880s on in order to employ Mach’s anti-metaphysics against his primary opponent, Wilhelm Ostwald’s energeticism. Boltzmann’s consistent empiricism had important consequences for the basic principles of physical science. In the last years of his life and especially in his 1903–1906 lectures on natural philosophy, he contemplated that even the law of energy conservation was only statistically valid—an idea that would surge much later in the 1924 Bohr-Kramers-Slater quantum theory—and that the entropy of a system might be described by a nowhere differentiable function. (Boltzmann 1898)

Exner amended Boltzmann’s late indeterminism in an important dimension. While Boltzmann had devoted surprisingly little attention to the interpretation of probability, Exner brought the relative frequency interpretation, or the *Kollektivmaßlehre*, developed by Gustav Theodor Fechner (1897) to bear on the kinetic theory of gases. On this basis, he could simultaneously claim that (*i*) in physics “we observe regularities which are brought out exclusively by chance” (Exner 1909, 13) but whose probability is so high “that it equals certainty for human conceptions” (Ibid., 16); while (*ii*) in the domain of the humanities and the descriptive sciences “the random single events succeed one another too slowly [such that] there can be no talk about a law.” (Ibid., 14) Still, or so he would claim in an unpublished manuscript (1923), the evolution of culture was shaped by the second law in virtue of which culture and science necessarily advance and spread despite the death of the individual cultural organism. Such read Exner’s own reaction to the Spenglerian challenge. (Cf. Hiebert 2000, Stöltzner 2002)

Let me turn to the opposite side in the first phase of the causality debate. Planck, in his famous Leiden lecture of 1908 that had started the polemics with Mach, vigorously defended what he took to be Boltzmann’s legacy against Mach’s anti-realism. In



1914, he now felt obliged to save Boltzmann's legacy from Exner's overinterpretation. Planck stressed "the fundamental importance of performing an exact and fundamental separation between ... the *dynamical*, strictly causal, and the merely *statistical* type of lawfulness for understanding the essence of all scientific knowledge." (1914, 57) This distinction finds its expression in the sharp contrast between reversible processes subsumed under a dynamical law and irreversible processes governed by the second law of thermodynamics. "This dualism ... to some may appear unsatisfactory, and one has already attempted to remove it—as it does not work out otherwise—by denying absolute certainty and impossibility at all and admitting only higher or lower degrees of probability. ... But such a view should very soon turn out to be a fatal and shortsighted mistake. (Ibid., 63) This was an obvious allusion to Exner, who responded to Planck's in a separate chapter of his 1919 *Lectures on the Physical Foundations of Natural Science*.

If we look at Planck's line of argument, we come to recognize that the principal difference between what I call Vienna Indeterminism and the Berlin reading of Boltzmann consisted in the relationship between causality and physical ontology. Either one followed, as did the Berliners, Kant by claiming that to stand in a causal relationship was a condition of the possibility for the reality of a physical object (Kant called this empirical realism), or one agreed with Mach that causality consisted in functional dependencies between the determining elements and that physical ontology was about 'facts' (*Tatsachen*) that consisted in stable complexes of such dependencies. To those standing in the Kantian tradition, the latter stance fell short of the aims of scientific inquiry. Those standing in the Hume-Mach tradition, however, had more leeway in searching for an ontology that was suitable for a new scientific theory. Notice that this difference in ontology extends across a larger historical time scale than the debate I am focusing on because it reached back to Mach's works of the 1870s and 1880s and ended only when philosophers of science abandoned the ideal of descriptivism after 1945.

Based upon this basic distinction between two notions of causality, Vienna Indeterminism—as touted by Exner in 1908—can be characterized by the following three commitments: (i) The highly *improbable events* admitted by Boltzmann's statistical derivation of the second law of thermodynamics exist. (ii) In a radically empiricist perspective, the burden of proof rests with the determinist who must provide a sufficiently specific theory of microphenomena before claiming victory over a merely statistical theory. Even worse, assuming a deterministic micro-theory without cogent reasons would lead to a "duplication of natural law [that] closely resembles the animistic duplication of natural *objects*." (Schrödinger 1929, 11)—as Schrödinger put it in his 1922 Zurich inaugural address. (iii) The only way to arrive at an empirical notion of objective probability is by way of the limit of relative frequencies. It is meaningful to assume the existence of statistical collectives (*Kollektivgegenstände*) and relate them to experience even though the limit is only obtained for infinitely large collectives. In 1912 and 1919, von Mises provided the rigid mathematical framework for the relative frequency interpretation.

Let me add that one has to distinguish two kinds of realism within the within the younger generation of Vienna Indeterminists. While Frank and von Mises came to elaborate the conventionalist picture and take theories as purely symbolic entities co-ordinated to experience, Schrödinger never abandoned Boltzmann's conception of theories as universal pictures.

In 1914, Planck rejected all three tenets of Vienna Indeterminism, but in the 1920s

he reconciled himself with the highly improbable events (*i*). But even after the advent of quantum mechanics, Planck still cherished the hope for a deterministic reformulation of atomic physics. His former student Moritz Schlick gradually approached Vienna Indeterminism as far as the burden of proof (*ii*) was concerned, but he never accepted the relative frequency interpretation (*iii*). Still in 1925, when already chairing the Vienna Circle's discussions, he held that "only in the utmost case of emergency will the scientist or philosopher decide to postulate purely statistical micro-laws, since the scope of such an assumption would be enormous: The principle of causality would be abandoned, ... and hence the possibility of exhaustive knowledge would have to be renounced." (Schlick 1925, 461/61) After the case of emergency had occurred in the form of quantum mechanics, Schlick (1931) presented an entirely new theory of causality in which the verificationist criterion of meaning blocked the assumption of a micro-world that was deterministic but unobservable in point of principle. But Schlick still demanded to separate all statistical regularity (*Gesetzmäßigkeit*) into strict law and pure randomness, such that there were strictly speaking no "statistical laws"—a thesis that surprised physicists as diverse as Einstein and Heisenberg. The reason was that Schlick till the end remained committed to Johannes von Kries's (1886) *Spielraumtheorie* of probability in which objective randomness was integrated into a deterministic Kantian universe. While Schlick had to openly revoke his 1920 theory of causality in the face of quantum mechanics, the Vienna Indeterminists could feel themselves confirmed. It is important for the sociological coherence of the latter tradition that they typically combined such a declaration with an explicit reference to Exner's priority, while Schlick held that Exner's works contained nothing beyond the traditional philosophical criticism against determinism.

The confrontation just sketched provides a framework, in which also other alleged 'converts to acausality' can be integrated. Here are just two examples. Walter Nernst, for one, had not forgotten the days he had worked with Boltzmann in Graz. "Among all laws [of physics] the thermodynamical ones occupy a distinctive position because unlike all others they are not just of a special kind, but applicable to any process one can imagine." (1922, 492) In the same vein, Exner had, in 1908, argued that the second law is the basic principle of nature. If one related all physical laws to the second law of thermodynamics, so Nernst continued, this would not reduce their significance or rank; "it would however put an end to the logical overuse of the laws of nature." (Ibid., 493)

In a review of Exner's (1919) *Lectures*, Hans Reichenbach endorsed "that Exner unequivocally advocates the objective meaning of the probabilistic laws in which he rightly conceives a very general regularity of nature." (Reichenbach 1921, 415) As did Exner, Reichenbach held that the basic laws of nature were of a statistical kind. But he did so for reasons that contradicted the radical empiricism of the Vienna Indeterminists. In his Ph.D. dissertation of 1915 and in a series of papers ensuing from it in the early 1920s, he argued that the principle of causality must be supplemented with a principle of lawful distributions (later called principle of the probability function) that guarantees that future empirical findings do not constantly change the form of the law. Due to the unavoidability of measurement errors the connection between our experiences and probability theory was of a more basic kind than the one between any other theory and our experiences. This thesis of Reichenbach became a source of conflict with von Mises.

I am afraid that I have to leave it at these sketchy remarks about the continuity of the causality debate across the breakdown of the two empires in 1918 and the quantum

revolution in 1926. Let me just add that the problem remained under philosophical dispute even at a time when most physicist had accepted quantum mechanics and Born's statistical interpretation of the wave function, and it did so even within the narrower circle of Logical Empiricists.

## The Physicist-Philosophers and Their Main Forum

Let me now turn to the sociological context of the causality debates. I have already emphasized the importance of the role model of physicist-philosopher for my case. Let me now describe how a physicist laid claim to this status, even though he might have remarked to his colleagues, cunningly or wittingly, that this represented only his Sunday's activity.

Forman was right to assume "that institutions of German academic life provided frequent occasions for addresses before university convocations", and that this indicates "the extraordinary heavy social pressure which the academic environment could and did exert upon the individual scholar and scientist placed within it." (1971, 6f.) Both in the Wilhelmin Empire and in the Weimar Republic, the main duty of a physicist having been elected rector, dean of the philosophical faculty, or secretary of an academy was to build a bridge to his colleagues from the humanities. They demanded something more profound than just popularizing one's scientific achievements and emphasizing their importance for technology and state.

Academic customs thus set the stage for the physicist-philosophers. The most influential role models were Hermann von Helmholtz and Ernst Mach, because it was mainly them who led the way out of the older *Naturphilosophie* by developing a new style of discussing the foundations of science as a philosophical problem. For this reason, many physicist-philosophers following in their footsteps remained critical towards excessive speculation, or published them anonymously and with a grain of salt, and they often eschewed entering into popular discourse. Quite a few of them, accordingly, regarded Wilhelm Ostwald's monistic sermons and Ernst Haeckel's writings with suspicion.

The publication of the academic addresses followed a typical scheme. Initially, they came out as separate booklets and were republished in one or two journals of the learned societies. At a certain point, a physicist would then assemble a collection of those academic speeches into a book that bore a title such as "Popular Writings" (Boltzmann 1905) or "Physical Panoramas" (Planck 1922). The publication of such a book testified the author's new status as a physicist-philosopher. There were also a few journals that combined publications of scientists having a philosophical thrust with papers penned by guided philosophers who were positively disposed towards the sciences, most prominently among them the *Vierteljahrsschrift für wissenschaftliche Philosophie und Soziologie* and Ostwald's *Annalen der Naturphilosophie*. They ceased publication in 1916 and 1921 respectively.

In 1913, the media landscape for the physicist-philosopher underwent a significant change. From now on, the mentioned academic addresses to a large percentage were published by the newly founded *Die Naturwissenschaften*. Modeled after the British *Nature*, the "scientific weekly for the progresses of science, medicine, and technology"—thus read its subtitle—strove to "follow the major developments within the whole of natural science and present them in a generally comprehensible and captivating form"

(1913, 1). The journal not only emphasized the unity of the sciences in a time of rapidly progressing specialization, but also—and this was among its most distinctive features as compared to *Nature*—the philosophical and cultural context of the sciences. To a large extent, this orientation was the product of the singular nature of Arnold Berliner, who ran the journal from 1913 until he was forced out in 1935 under the Nuremberg laws. Berliner was both one of the early technical physicist, who had worked as a factory director, and a “*Kultur Mensch*”, who venerated Goethe and was one of Gustav Mahler’s closest friends. From the recollections of Wilhelm Westphal (1952) we learn that for the younger Berlin physicists Berliner was an intellectual father figure not unlike what Exner had become for his circle.

The impressive number of philosophical articles solicited by Berliner can be divided into two groups. On the one hand, he ran a kind of education program by publishing survey papers on Goethe, Kant, Schopenhauer, etc. On the other hand, he published papers in which scientists reflected on the conceptual and philosophical foundations of their most recent achievements, among them most papers of the causality debate and many papers and reviews penned by Logical Empiricists. Conversely, until 1930 those Logical Empiricists who had a science background published roughly a third of their papers in *Die Naturwissenschaften*. (For further figures, see Stöltzner (2000).) This proves that among the readers of this journal neo-positivism was by far less fringy than Forman assumed.

Berliner’s journal unequivocally took sides in two debates that were of great importance for science as a whole in the early years of the Weimar republic. First, in the struggles about relativity theory that had intensified after 1918, *Die Naturwissenschaften* became an important stronghold in the “defense belt” (Hentschel 1990) around Einstein. This debate shaped the philosophical understanding of modern physics, be it relativistic or quantum, and prompted physicist-philosophers to take a stand against public accusations.

Second, Berliner’s journal devoted two papers to a severe criticism of Oswald Spengler’s views on biology and physics. One of the critics, the applied mathematician Paul Riebesell, had already participated in the relativity debates. (Riebesell 1916) As did the Vienna Indeterminists, Riebesell accepted statistical laws as genuine laws. This even permitted him to turn the tables against Spengler. “Science—not the philosophy of nature—will now as before stick to the principle of causality and will approach precisely Spengler’s problem of the predetermination of history with its new methods. For, by means of statistical laws—which *Spengler* incidentally does not recognize as mathematical laws—one has already successfully analyzed those mass phenomena, which historical questions are all about.” (Riebesell 1920, 508) Thus Riebesell drew terminological consequences from the present state of physics and the social sciences, but not in an act of adaptation. In a certain sense, the break between Spengler’s cultural morphology and the quantitative social science mentioned by Riebesell was even more radical than the one between Spengler’s concept of causality and statistical mechanics.

In evaluating the sociological impact of this confutation of Spengler for the German scientific community, we have to consider that *Die Naturwissenschaften* was closely connected to two leading research organizations of the German-speaking world, the *Deutsche Gesellschaft der Naturforscher und Ärzte* and the *Kaiser-Wilhelm-Gesellschaft*. In virtue of this authoritative character, I have considered (Stöltzner 2000, 2005) *Die Naturwis-*

*senschaften* as a scientifically modernist submilieu that provided scientists with a cultural identity more specific than just being *Bildungsbürger*, such that they did not face the general milieu directly without a stabilizing group identity. Today, however, I believe that the concept of milieu—even in the operationalist sense of Fleck (1929)—is too un-specific and ultimately forces us to accept the alternative that Forman had posed at the beginning of his study, to wit, retrenchment versus adaptation. To my taste, all this sounds too passive for physicist-philosophers. Moreover, after 1900 there existed no longer a homogeneous intellectual milieu that could, as a whole, change under the influence of the lost war. As I will outline in the final section, one has to take a multi-layered approach instead. Thus I would now say that *Die Naturwissenschaften* simply provided a forum for those who endorsed scientific modernism, which could mean different things in different disciplines, and considered science as an integral part of the general culture, towards which scientists heeded different attitudes. Much of this orientation of *Die Naturwissenschaften*, especially in the fields of physics and philosophy, was due to the singular nature of Arnold Berliner and his embedding into the Berlin scientific elite.

A characteristic element of the conduit of physicist-philosophers was, a few notable exceptions notwithstanding, their independence from ruling philosophical schools. This permitted them to form strategic alliances. Let me first provide an abstract characterization of this notion. A strategic alliance was formed if there was a set of basic philosophical convictions that a group of physicists considered as central in order to further their philosophical agenda within a particular intellectual, social or disciplinary context. In this case, they confined their disagreements to internal discussions, even though in retrospect these may appear substantial. Strategic alliances dissolved and their members regrouped, as the convictions considered pivotal within the respective context underwent changes. It is important to stress that the philosophical ambitions of a physicist-philosopher were not exhausted by the intersection constituting this strategic alliance. Or to cast it into Fleckian terms, the members of a strategic alliance were typically members of different thought collectives.

It seems to me that both Logical Empiricism, at least initially, and the Göttingen-Copenhagen interpretation of quantum mechanics represented strategic alliances of this kind. When Logical Empiricists joined up with the latter, the tradition of Vienna Indeterminism ended in the mid 1930s because this move alienated Schrödinger from Frank and von Mises. The reasons were at least twofold. For one, Logical Empiricists decided to combat the metaphysical misinterpretations of quantum theory by developing an empiricist reading of Bohr's complementarity. To do so they invoked a verificationist criterion of meaning that, in its language-oriented version, was unacceptable to Schrödinger who sought for universally valid pictures rather than concepts with a limited domain of applicability. More generally, after the EPR-paper of 1935 and Schrödinger's (1935) cat paper, the discussions about the interpretation of quantum mechanics shifted from causality and indeterminism to questions of reality in the atomic domain.

But there was also a sociological element. By organizing specific meetings, through the foundation of their own journal *Erkenntnis*, with their search for international allies, and through a debate whether their distinctive method consisted in the logic of science (Carnap), scientific philosophy (Reichenbach), or encyclopedism (Neurath), Logical Empiricists after 1930 accomplished the basic steps in establishing a new scientific discipline. Through this process of discipline formation, the role model of physicist-philosopher, al-

beit still existing, lost its pervasiveness in the German-speaking world. The further course of the new discipline “philosophy of science” was not to be without implications for how the Forman thesis was cast.

### Contextualizing the Forman Thesis

In this section, I first want to show that the Forman thesis is a child of its days in more than one respect; not only by revealing a strong, or even causal, influence of social factors on the conceptual structure of empirical science—a perspective that would prove most influential during the 1970s and beyond. Forman’s treatment of the relationship between physical theory and cultural milieu was also deeply informed by what was common to both Rudolf Carnap’s philosophy of science and Thomas S. Kuhn’s revolutionist perspective on the historiography of science. As did most members of their respective disciplines, both focused on theory and in doing so they treated a scientific theory as a single and largely homogeneous entity. This, so I claim, prevented Forman and others from conceiving the causality debate in its larger historical context and its proper discursive mode, and made him disregard the philosophical continuities beyond how the protagonists of his study, after 1918, used philosophical keywords, such as ‘causality’, ‘crisis’ and ‘Spengler’.

In the famous debates with W.V. Quine, Carnap (1950) had argued that questions about the existence of scientific objects were only meaningful once a linguistic framework had been specified. While Carnap continued to hold that the choice of a framework was guided by pragmatic concerns, Kuhn’s (1962) *Structure of Scientific Revolutions* pointed out that at certain moments in history, scientific revolutions overthrew an old conceptual framework and instated a new one. The main point of Kuhn’s argument, at least in its original form, was that the old and new frameworks were incommensurable, such that there was no rational bridge from one paradigm to the other. Kuhn’s book has often been understood as the final blow to a philosophy of science in the Vienna Circle style even though it had received Carnap’s endorsement. For, both agreed that there existed not meta-framework that could justify the transitions between two frameworks as rational. Their main difference was that Carnap denied strong versions of the theory-ladenness of observation, such that the brute facts always provided a bridge between two paradigms even if there was no theoretical bridge between the old and the new paradigm. Both their consensus and disagreement hence concerned the relationship between one or two theories and unstructured empirical data.

The subsequent debate among philosophers centered around whether the history of science could be rationally reconstructed—as Lakatos and Popper held—or whether it was essentially contingent—as Feyerabend came to radicalize Kuhn’s analysis. This debate was still in its early phase when Forman’s paper came out. Seen from perspective of the philosophical frontline between Lakatos and Feyerabend in its mature form, we find an interesting ambiguity in Forman’s thesis. On the one hand, by claiming a causal influence of the post-war milieu he argued in favor of historical contingency in the style of Feyerabend. On the other hand, Forman held that after 1927 there was sufficient reason to abandon causality and thus assumed, in contrast, the rationality of scientific development. Forman, it becomes clear, was not a social constructivist.

In her *Quantum Dialogue*, Mara Beller (1999) has made the case that Forman’s thesis

parallels the Kuhnian picture and that he accordingly has written the history of the winners. On her account, it was mainly Bohr's power politics that changed a fruitful continuous dialogue into a revolutionary narrative. In the form of deBroglie's pilot wave theory, she stressed, the possibility of a causal quantum mechanics had always existed. While I agree with Beller's paralleling Forman and Kuhn, I doubt that the radical counterposition between dialogical emergence and rhetorical consolidation—so the two parts of her book—does justice to the rather stable philosophical convictions of the protagonists of her narrative because it downgrades them to justificatory rhetoric.

Again motivated by the deBroglie-Bohm theory, Jim Cushing (1994) has rightly interpreted quantum mechanics as a case of Duhemian underdetermination. But he additionally construed a counterfactual history showing how the causal picture could have prevailed, filing thus an equal rights claim for alternative interpretations of quantum mechanics. This move was justly criticized among others by Beller (1999) and Forman (1995). Once again, we find the above-mentioned confrontation between one or two theories and empirical data. No wonder that Cushing stressed that philosophical motives were of little importance, apart perhaps from positivism's role in justifying the Copenhagen dogma. Both Beller and Cushing identify philosophy with guided or academic philosophy and thus miss the peculiar role model of physicist-philosopher that lies at the heart of my reconstruction of the causality debate.

It seems to me, in contrast to Forman, Beller and Cushing, that the causality debates among German physicist-philosophers can only be assessed by departing from a multi-layered structure of beliefs and attitudes encompassing general philosophical principles, mathematical formalisms, specific theories, personal research agendas and cultural self-identities that evolved and changed on different time scales. Let me integrate my story into this picture.

I have claimed that the causality debate extended across roughly three decades, from Exner's 1908 inaugural address until the discussions ensuing from the EPR-paper. There was one thought collective, Vienna Indeterminism, whose members were not forced to change their philosophical principles, neither in 1918, when a deep political crisis began, nor in the face of the growing problems in atomic physics that had started around 1920, nor after the recognition of the strange features of the new quantum theory that Born's interpretation of the wave function brought to light. In Schlick's case we have seen that for those who, unlike Schrödinger, fully endorsed the new quantum mechanics, the philosophical reorientation was eased by the fact that indeterminism had already been an option widely discussed. If we look at physicist-philosophers, such as Frank, von Mises and Schlick, we see that the orientation at a Machian or Kantian conception of causality, that lives on an even longer time scale, proved to be an enormously stable philosophical disposition. Schlick, in particular, needed much longer to abandon the Kantian category of causality than he did for those of space and time in the context of relativity theory.

I have remained largely silent about the mathematical levels involved in my story. But I have to mention at least one of them, not least because it demonstrates that I am not writing a winners' history myself. In spite of the important role of probability for the causality debate, the most important breakthrough in the field came only in 1932 with Kolmogorov's axiomatization that in virtue of its abstract nature avoided the problems that plagued Fechner's and von Mises's statistical collectives. (See Hochkirchen 1999) This achievement only made clear that the problem of quantum probabilities

was not fully resolved and that a full-blown frequentism as advocated by the Vienna Indeterminists does not do the job.

It remains to be seen at further historical examples whether the higher-level principles in the above structure, the philosophical and the mathematical ones, may exert such a strong force on concept formation that they can be considered historically relativized a priori, as Michael Friedman (2001) has suggested in order to save the Kuhnian insight from social constructivism, or whether they only mediate across fractures in the conceptual development that occur on another level. The latter claim, it seems to me, can be reconciled with Fleck's (1935) insight that a single scientist may simultaneously belong to different thought collectives. Such was the tack taken in the present analysis because it permitted me to incorporate also other thinkers, such as Reichenbach and Nernst, who neither were part of Vienna Indeterminism nor shared Planck's insistence of determinism or Schlick's separation between lawfulness and randomness.

Finally, it is important to note that the existence of local traditions, such as Vienna Indeterminism, does not contradict the integrity of the causality debate and the debates occurring in *Die Naturwissenschaften* in so far as they took place within a single but multifarious German-speaking scientific culture. For this reason, I am happy to observe that Forman considers the Vienna tradition no longer just as a "subterranean anticausality current" (Forman 1971, 67) but as part of a broader Austro-Hungarian tradition in which positivist tendencies were pivotal and which had its roots long before 1918. (Forman 2007, 40) I hope to have shown that also the stance of the Weimar participants in the debate—both thematically and socially—was not primarily a product of the fall of the Wilhelminian Empire but shaped by earlier philosophical commitments that had been defined in a struggle about Boltzmann's legacy statistical mechanics.

*Acknowledgements:* I am greatly indebted to Veronika Hofer for many discussions about historical methodology, including intellectual milieus and Fleckian thought collectives, and a critical reading of the present paper. This paper has emerged from a talk at the Conference "The Cultural Alchemy of the Exact Sciences: Revisiting the Forman Thesis" held at the University of British Columbia, Vancouver, BC, Canada, in March 2007 and was revised for presentation at the HQ1-conference at the Max-Planck-Institute in Berlin. I thank the organizers and participants of both conferences for their very helpful questions and remarks.

### References:

- Beller, Mara (1999), *Quantum Dialogue. The Making of a Revolution*, The University of Chicago Press, Chicago.
- Boltzmann, Ludwig (1898), 'Über die sogenannte H-Kurve', *Mathematische Annalen* **50**, 325–332.
- Boltzmann, Ludwig (1905), *Populäre Schriften*, J.A. Barth, Leipzig; partially translated in: *Theoretical Physics and Philosophical Problems*, ed. by Brian McGuinness, Reidel, Dordrecht, 1974.
- Carnap, Rudolf (1950), 'Empiricism, Semantics, and Ontology', *Revue internationale de philosophie* **4**, 20–40.



- Cushing, James T. (1994), *Quantum Mechanics—Historical Contingency and the Copenhagen Hegemony*, Chicago University Press, Chicago.
- DuBois-Reymond, Emil (1872), *Über die Grenzen des Naturerkennens*, Leipzig: Veit.
- Exner, Franz S. (1909), *Über Gesetze in Naturwissenschaft und Humanistik*, Alfred Hölder, Wien-Leipzig.
- Exner, Franz S. (1919), *Vorlesungen über die physikalischen Grundlagen der Naturwissenschaften*, Franz Deuticke, Leipzig-Wien.
- Exner, Franz S. (1923), *Vom Chaos zur Gegenwart*, unpublished mimeographed typescript.
- Fechner, Gustav Theodor (1897), *Kollektivmaßlehre*, im Auftrag der Königlich Sächsischen Gesellschaft der Wissenschaften, herausgegeben von Gottlob Friedrich Lipps, Leipzig: W. Engelmann.
- Fleck, Ludwik (1929), ‘Zur Krise der ‘Wirklichkeit’’, *Die Naturwissenschaften* **17**, 425–430.
- Fleck, Ludwik (1935), *Entstehung und Entwicklung einer wissenschaftlichen Tatsache. Einführung in die Lehre vom Denkstil und Denkkollektiv*, Basel 1935.
- Forman, Paul (1971), ‘Weimar Culture, Causality, and Quantum Theory, 1918–1927: Adaption by German Physicists and Mathematicians to a Hostile Intellectual Environment’, *Historical Studies in the Physical Sciences* **3**, 1–114.
- Forman, Paul (1984), ‘Kausalität, Anschaulichkeit, and Individualität, or How Cultural Values Prescribed the Character and the Lessons Ascribed to Quantum Mechanics’, in: Stehr, Nico and Meja, Volker (eds.), *Society and Knowledge. Contemporary Perspectives in the Sociology of Knowledge*, Transaction Books, New-Brunswick-London, 333–347.
- Forman, Paul (1995), Review of Quantum Mechanics. Historical Contingency and the Copenhagen Hegemony by James T. Cushing, *Science* **267**, 1844 (24 March 1995).
- Forman, Paul (2007), ‘Die Naturforscherversammlung in Nauheim im September 1920’, in: Dieter Hoffmann and Mark Walker (eds.), *Physiker zwischen Autonomie und Anpassung. Die Deutsche Physikalische Gesellschaft im Dritten Reich*, Weinheim: VCH-Wiley, 29–58.
- Friedman, Michael (2001), *Dynamics of Reason*, Stanford: CSLI Publications.
- Frank, Philipp (1929), ‘Was bedeuten die gegenwärtigen physikalischen Theorien für die allgemeine Erkenntnislehre’, *Die Naturwissenschaften* **17**, 971–977 & 987–994; also in: *Erkenntnis* **1**, 126–157. English translation ‘Physical Theories of the Twentieth Century and School Philosophy’, in (Frank, 1961), 96–125.
- Frank, Philipp (1932), *Das Kausalgesetz und seine Grenzen*, Vienna: Springer; English translation *The Law of Causality and Its Limits*, Dordrecht: Kluwer, 1998.

## The Causality Debates of the Interwar Years and their Preconditions

---

- Hentschel, Klaus (1990), *Interpretationen und Fehlinterpretationen der speziellen und der allgemeinen Relativitätstheorie durch Zeitgenossen Albert Einsteins*, Basel, Birkhäuser.
- Hendry, John (1980), 'Weimar Culture and Quantum Causality', *History of Science* **18**, 155–180.
- Hiebert, Erwin N. (2000), 'Common Frontiers of the Exact Sciences and the Humanities,' *Physics in Perspective* **2**, 6–29.
- Hochkirchen, Thomas (1999), *Die Axiomatisierung der Wahrscheinlichkeitsrechnung und ihre Kontexte: von Hilberts sechstem Problem zu Kolmogoroffs Grundbegriffen*, Göttingen: Vandenhoeck & Ruprecht.
- Kuhn, Thomas S. (1962), *the Structure of Scientific Revolutions*, University of Chicago Press, Chicago, IL.
- Kries, Johannes von (1886), *Prinzipien der Wahrscheinlichkeitsrechnung*, Mohr, Freiburg i.B., Second edition with a new foreword 1927.
- Mises, Richard von (1912), 'Über die Grundbegriffe der Kollektivmaßlehre', *Jahresbericht der Deutschen Mathematiker-Vereinigung* **21**, 9–20.
- Mises, Richard von (1919), 'Fundamentalsätze der Wahrscheinlichkeitsrechnung', *Mathematische Zeitschrift* **5**, 52–99 & 100.
- Mises, Richard von (1930), 'Über kausale und statistische Gesetzmäßigkeit in der Physik', *Die Naturwissenschaften* **18**, 145–153; also in: *Erkenntnis* **1**, 189–210.
- Nernst, Walter (1922a), 'Zum Gültigkeitsbereich der Naturgesetze', *Die Naturwissenschaften* **10**, 489–495.
- Planck, Max (1914), 'Dynamische und statistische Gesetzmäßigkeit', in: *Wege zur physikalischen Erkenntnis*, S. Hirzel, Leipzig, 1944, 54–67.
- Planck, Max (1922), *Physikalische Rundblicke*, Leipzig, Barth.
- Reichenbach, Hans (1921), Rezension von 'Exner, Franz, Vorlesungen über die physikalischen Grundlagen der Naturwissenschaften', *Die Naturwissenschaften* **9**, 414–415.
- Riebesell, Paul (1916), 'Die Beweise für die Relativitätstheorie', *Die Naturwissenschaften* **4**, 98–101.
- Riebesell, Paul (1918), 'Die neueren Ergebnisse der theoretischen Physik und ihre Beziehungen zur Mathematik', *Die Naturwissenschaften* **6**, 61–65.
- Riebesell, Paul (1920), 'Die Mathematik und die Naturwissenschaften in Spenglers 'Untergang des Abendlandes', *Die Naturwissenschaften* **8**, 507–509.
- Schlick, Moritz (1920), 'Naturphilosophische Betrachtungen über das Kausalprinzip', *Die Naturwissenschaften* **8**, 461–474, English translation in *Philosophical Papers*, ed. by Henk Mulder and Barbara F. B. van de Velde-Schlick, Reidel, Dordrecht, vol. I, pp. 295–321.

- Schlick Moritz (1925), *Naturphilosophie*, in Max Dessoir (ed.): *Lehrbuch der Philosophie: Die Philosophie in ihren Einzelgebieten*, Ullstein, Berlin, pp. 397–492; English translation: *Philosophical Papers*, ed. by Henk Mulder and Barbara F.B. van de Velde-Schlick, Reidel, Dordrecht, vol. II, pp. 1–90.
- Schlick, Moritz (1931), ‘Die Kausalität in der gegenwärtigen Physik’, *Die Naturwissenschaften* **19**, 145–162; English translation in *Philosophical Papers*, vol. II, 176–209.
- Schrödinger, Erwin (1922), ‘Was ist ein Naturgesetz?’, *Die Naturwissenschaften* **17** (1929), 9–11;
- Schrödinger, Erwin (1935), ‘Die gegenwärtige Situation in der Quantenmechanik’, *Die Naturwissenschaften* **23**, 807–812 & 823–828 & 844–849.
- Sommerfeld, Arnold (1929), ‘Einige grundsätzliche Bemerkungen zur Wellenmechanik’, *Physikalische Zeitschrift* **30**, 866–870.
- Stöltzner, Michael (1999). “Vienna Indeterminism: Mach, Boltzmann, Exner”, *Synthese* **119**, 85–111.
- Stöltzner, Michael (2000) “Kausalität in *Die Naturwissenschaften*. Zu einem Mi-lieuproblem in Formans These”, in: Heike Franz, Werner Kogge, Torger Möller, Torsten Wilholt (eds.), *Wissensgesellschaft: Transformationen im Verhältnis von Wissenschaft und Alltag*, pp. 85–128. (*iwt-paper 2000*, accessible under <http://archiv.ub.uni-bielefeld.de/wissensgesellschaft/publikationen/Michael%20Stoeltzner%20Wissensgesellschaft.pdf>).
- Stöltzner, Michael (2002), “Franz Serafin Exner’s Indeterminist Theory of Culture”, *Physics in Perspective* **4**, 267–319.
- Stöltzner, Michael (2003), “Vienna Indeterminism II: From Exner to Frank and von Mises”, in: P. Parrini, W. Salmon, M. Salmon (eds.): *Logical Empiricism. Historical and Contemporary Perspectives*, Pittsburgh: University of Pittsburgh Press, 194–229.
- Stöltzner, Michael (2005), *Vienna Indeterminism. Causality, Realism and the Two Strands of Boltzmann’s Legacy*, Ph.D.-dissertation, University of Bielefeld, March 2003. Publication in preparation; accessible under <http://bieson.ub.uni-bielefeld.de/volltexte/2005/694/>
- Westphal, Wilhelm (1952), ‘Arnold Berliner zum Gedächtnis’, *Physikalische Blätter* **8**, 121.

# 8 Electron Spin or ‘Classically Non-Describable Two-Valuedness’

DOMENICO GIULINI

*In December 1924 Wolfgang Pauli proposed the idea of an inner degree of freedom of the electron, which he insisted should be thought of as genuinely quantum mechanical in nature. Shortly thereafter Ralph Kronig and a little later Samuel Goudsmit and George Uhlenbeck took up a less radical stance by suggesting that this degree of freedom somehow corresponded to an inner rotational motion, though it was unclear from the very beginning how literal one was actually supposed to take this picture, since it was immediately recognised (already by Goudsmit and Uhlenbeck) that it would very likely lead to serious problems with Special Relativity if the model were to reproduce the electron’s values for mass, charge, angular momentum, and magnetic moment. However, probably due to the then overwhelming impression that classical concepts were generally insufficient for the proper description of microscopic phenomena, a more detailed reasoning was never given. In this contribution I shall investigate in some detail what the restrictions on the physical quantities just mentioned are, if they are to be reproduced by rather simple classical models of the electron within the framework of Special Relativity. It turns out that surface stresses play a decisive role and that the question of whether a classical model for the electron does indeed contradict Special Relativity can only be answered on the basis of an exact solution, which has hitherto not been given.*

## 8.1 Introduction

The discovery of electron spin is one of the most interesting stories in the history of Quantum Mechanics; told e.g. in van der Waerden’s contribution to the Pauli Memorial Volume ([11], pp. 199–244), in Tomonaga’s book [46], and also in various first-hand reports [47,19,30]. This story also bears fascinating relations to the history of understanding Special Relativity. One such relation is given by Thomas’ discovery of what we now call “Thomas precession” [44,45], which explained for the first time the correct magnitude of spin-orbit coupling and hence the correct magnitude of the fine-structure split of spectral lines, and whose mathematical origin can be traced to precisely that point which marks the central difference between the Galilei and the Lorentz group (this is e.g. explained in detail in Sects. 4.3–4.6 of [17]). In the present paper I will dwell a little on another such connection to Special Relativity.

As is widely appreciated, Wolfgang Pauli is a central figure, perhaps *the* most central figure, in the story of spin. Being the inventor of the idea of an inner (quantum mechanical) degree of freedom of the electron, he was at the same time the strongest opponent to attempts to relate it to any kind of interpretation in terms of kinematical concepts

that derive from the picture of an extended material object in a state of rotation. To my knowledge, Pauli's hypothesis of this new intrinsic feature of the electron, which he cautiously called "a classical non-describable two valuedness", was the first instance where a quantum-mechanical degree of freedom was claimed to exist without a corresponding classical one. This seems to be an early attempt to walk without the crutches of some 'correspondence principle'. Even though the ensuing developments seem to have re-installed—mentally at least—the more classical notion of a spinning electron through the ideas of Ralph Kronig (compare section 4 of van der Waerden's contribution to [11], pp. 209–216) and, a little later, Samuel Goudsmit and George Uhlenbeck<sup>1</sup>[20,21], Pauli was never convinced, despite the fact that he lost the battle against Thomas<sup>2</sup> and declared "total surrender" in a letter to Bohr written on March 12. 1926 ([27], Vol.I, Doc.127, pp.310). For Pauli the spin of the electron remained an abstract property which receives its ultimate and irreducible explanation in terms of group theory, as applied to the subgroup<sup>3</sup> of spatial rotations (or its double cover) within the full symmetry group of space-time, may it be the Galilei or the Lorentz group (or their double cover).<sup>4</sup> In this respect, Pauli's 1946 Nobel Lecture contains the following instructive passage (here and throughout this paper I enclose my annotations to quotes within square brackets):

Although at first I strongly doubted the correctness of this idea [of the electron spin in the sense of Kronig, Goudsmit and Uhlenbeck] because of its classical-mechanical character, I was finally converted to it by Thomas' calculations on the magnitude of doublet splitting. On the other hand, my earlier doubts as well as the cautious expression «classically non-describable two-valuedness» experienced a certain verification during later developments, since Bohr was able to show on the basis of wave mechanics that the electron spin cannot be measured by classically describable experiments (as, for instance, deflection of molecular beams in external electromagnetic fields) and

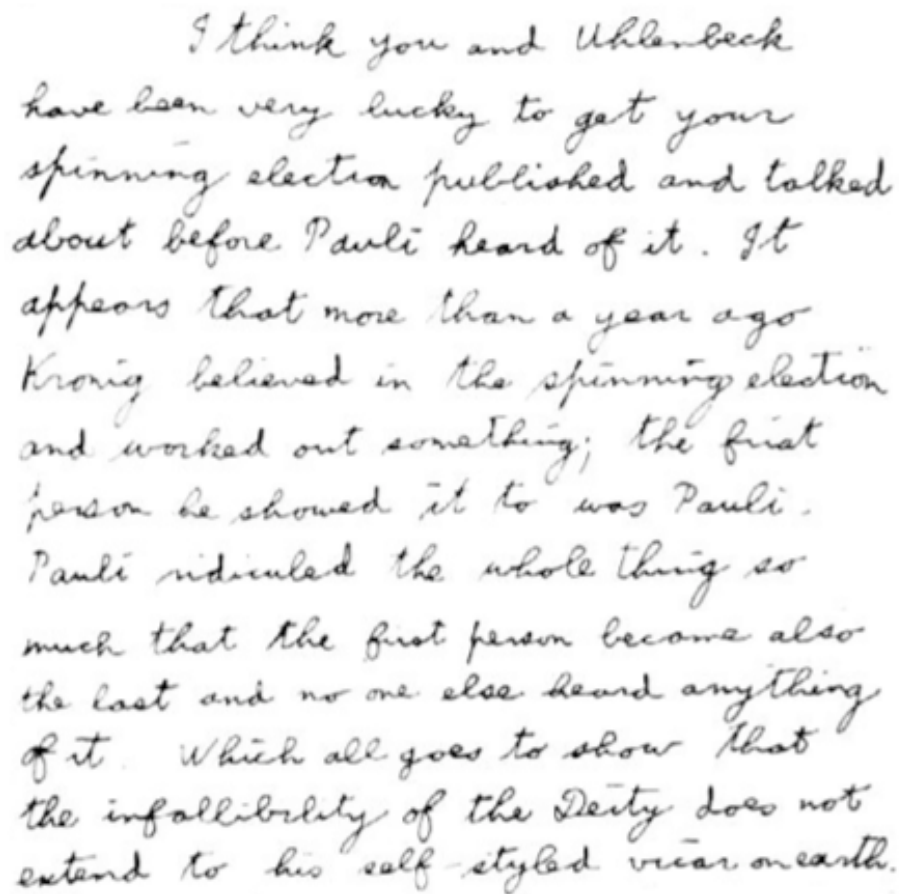
---

<sup>1</sup> Van der Waerden states that Goudsmit and Uhlenbeck conceived the idea of the spinning electron independently of Kronig, even though he also reports that after Kronig first told his idea to Pauli, who did not approve, in Tübingen on January 8th 1925 he went straight to Copenhagen to "discuss the problem with Heisenberg, Kramers and others", who did not approve either ([11], p.212). Hence, in principle, Kronig's idea could well have transpired to Goudsmit and Uhlenbeck prior to their publication, though there seems to be no evidence for that. In contrast, already in the spring of 1926 Kronig published two critical notes [26,25] in which he much stressed the problems with Goudsmit's and Uhlenbeck's idea (sic!). He concluded [26] by saying: "The new hypothesis, therefore, appears rather to effect the removal of the family ghost from the basement to the sub-basement, instead of expelling it definitely from the house." In later recollections he gently brings himself back into the game, like in his contribution to the Pauli memorial volume ([11], p.5–39), but also emphasises his awareness of the critical aspects, as, e.g., in a letter to van der Waerden ([11], p.212).

<sup>2</sup>At this point Frenkel's remarkable contribution [14] should also be mentioned, which definitely improves on Thomas' presentation and which was motivated by Pauli sending Frenkel Thomas' manuscript, as Frenkel acknowledges in footnote 1 on p.244 of [14]. A more modern account of Frenkel's work is given in [43].

<sup>3</sup>It is more correct to speak of the conjugacy class of subgroups of spatial rotations, since there is no (and cannot be) a single distinguished subgroup group of 'spatial' rotations in Special Relativity.

<sup>4</sup>Half-integer spin representations only arise either as proper ray-representations (sometimes called 'double-valued' representations) of spatial rotations  $SO(3)$  or as faithful true representations (i.e. 'single-valued') of its double-cover group  $SU(2)$ , which are subgroups of the Galilei and Lorentz groups or their double-cover groups respectively.

A handwritten note in cursive ink on a light background. The text is a letter from L.H. Thomas to S. Goudsmit, dated March 25th 1926. The handwriting is fluid and somewhat slanted. The text describes how Thomas' work on electron spin was published before Pauli's reaction, and how Kronig's earlier work was dismissed by Pauli, leading to the idea of spin being suppressed.

I think you and Uhlenbeck  
have been very lucky to get your  
spinning electron published and talked  
about before Pauli heard of it. It  
appears that more than a year ago  
Kronig believed in the spinning electron  
and worked out something; the first  
person he showed it to was Pauli.  
Pauli ridiculed the whole thing so  
much that the first person became also  
the last and no one else heard anything  
of it. Which all goes to show that  
the infallibility of the Deity does not  
extend to his self-styled vicar on earth.

Figure 8.1: Part of a letter by L.H. Thomas to S. Goudsmit dated March 25th 1926, taken from [18].

must therefore be considered as an essential quantum-mechanical property of the electron.<sup>5</sup> ([31], p. 30)

This should clearly not be misunderstood as saying that under the impression of Thomas' calculations Pauli accepted spin in its 'classical-mechanical' interpretation. In fact, he kept on arguing fiercely against what in a letter to Sommerfeld from December 1924 he called "model prejudices" ([27], Vol. I, Doc. 72, p. 182) and did not refrain from ridiculing the upcoming idea of spin from the very first moment (cf. Fig. 8.1). What

<sup>5</sup>At this point Pauli refers to the reports of the Sixth Physics Solvay Conference 1932. In his handbook article on wave mechanics, Pauli is more explicit ([33], p. 165): *The spin-moment of the electron can never be measured in clean separation from the orbital moment by those experiments to which the classical notion of particle-orbit applies.* (German original: "Das Spinmoment des Elektrons kann niemals, vom Bahnmoment eindeutig getrennt, durch solche Versuche bestimmt werden, auf die der klassische Begriff der Partikelbahn anwendbar ist.") However, this general statement seems to be based entirely on its validity in specific situations, like those discussed by Mott ([29], Appendix, pp. 440–442). A closer examination shows that the envisaged theorem of Bohr and Pauli is physically unwarranted in the generality in which it is presented above. This can, for example, be illustrated by the possibility to create macroscopically separated beams of polarised (anti)protons in a storage ring via the Stern-Gerlach effect (see [36]). Other examples to the same effect of Gedanken- and real experiments are discussed in [8].

Pauli accepted was the idea of the electron possessing an intrinsic magnetic moment and angular momentum, the latter being interpreted *exclusively* in a formal fashion through its connection with the generators of the subgroup of rotations within the Lorentz group, much like we nowadays view it in modern relativistic field theory. To some extent it seems fair to say that, in this case, Pauli was a pioneer of the modern view according to which abstract concepts based on symmetry-principles are seen as primary, whereas their concrete interpretation in terms of localised material structures, to which e.g. the kinematical concept of ‘rotation’ in the proper sense applies, is secondary and sometimes even dispensable. But one should not forget that this process of emancipation was already going on in connection with the notion of classical fields, as Einstein used to emphasise, e.g., in his 1920 Leiden address “Ether and the Theory of Relativity”<sup>6</sup> ([42], Vol. 7, Doc. 38, pp. 308–320). We will come back to this point below.<sup>7</sup>

Besides being sceptical in general, Pauli once also made a *specific* remark as to the inadequateness of classical electron models; that was three years after Thomas’ note, in a footnote in the addendum to his survey article “General Foundations of the Quantum Theory of Atomic Structure”<sup>8</sup>, that appeared 1929 as chapter 29 in ‘Müller-Pouillet’s Lehrbuch der Physik’. There he said:

Emphasising the kinematical aspects one also speaks of the ‘rotating electron’ (English ‘spin-electron’). However, we do not regard the conception of a rotating material structure to be essential, and it does not even recommend itself for reasons of superluminal velocities one then has to accept. ([24], Vol. 1, pp. 721–722, footnote 2)

Interestingly, this is precisely the objection that, according to Goudsmit’s recollections [18], Lorentz put forward when presented with Goudsmit’s and Uhlenbeck’s idea by Uhlenbeck, and which impressed Uhlenbeck so much that he asked Ehrenfest for help in withdrawing the already submitted paper [18]. He did not succeed, but the printed version contains at least a footnote pointing out that difficulty:

The electron must now assume the property (a) [a  $g$ -factor of 2], which LANDÉ attributed to the atom’s core, and which is hitherto not understood. The quantitative details may well depend on the choice of model for the electron. [...] Note that upon quantisation of that rotational motion [of the spherical hollow electron], the equatorial velocity will greatly exceed the velocity of light. ([20], p. 954)

This clearly says that a classical electron model cannot reproduce the observable quantities, mass, charge, angular momentum, and magnetic moment, without running into severe contradictions with Special Relativity.<sup>9</sup> The electron model they had in mind

---

<sup>6</sup>German original: Äther und Relativitätstheorie.

<sup>7</sup>The case of a classical electromagnetic field is of particular interesting insofar as the suggestive picture provided by Faraday’s lines of force, which is undoubtedly helpful in many cases, also provokes to view these lines as objects in space, like ropes under tension, which can be attributed a variable state of motion. But this turns out to be a fatal misconception.

<sup>8</sup>German original: Allgemeine Grundlagen der Quantentheorie des Atombaues.

<sup>9</sup>The phrase “upon quantisation” in the above quotation is to be understood quantitatively, i.e. as “upon requiring the spin angular-momentum to be of magnitude  $\hbar/2$  and the magnetic moment to be one magneton ( $g = 2$ )”.

was that developed by Abraham in his 1903 classic paper on the “Principles of Electron Dynamics” [1] (cited in footnote 2 on p. 954 of [20]). Interestingly, one of the first ones to spread this criticism was Kronig, who in [26] asserts that “the internal velocities would have to be exceedingly close to that of light” and again in [25] that “the velocities of spin would have to be exceedingly high if classical concepts could still be applied to the case in question” ([25], p. 329). Much later, in his letter to van der Waerden that we already mentioned, he again stresses as one of the primary difficulties with this idea “the necessity to assume, for the rotating charge of an electron of classical size, velocities surpassing the velocity of light” ([11], p. 212). Since then it has become standard textbook wisdom that classical electron models necessarily suffer from such defects (compare, e.g., [5], p. 155) and that, even in quantum mechanics, “the idea of the rotating electron is not to be taken literally”, as Max Born once put it ([5], p. 188). Modern references iterate this almost verbatim:

The term ‘electron spin’ is not to be taken literally in the classical sense as a description of the origin of the magnetic moment described above. To be sure, a spinning sphere of charge can produce a magnetic moment, but the magnitude of the magnetic moment obtained above cannot be reasonably modelled by considering the electron as a spinning sphere.

(Taken from  $\langle$  <http://hyperphysics.phy-astr.gsu.edu/hbase/spin.html> $\rangle$ )

In this contribution I wish to scrutinise the last statement. This is not done in an attempt to regain respect for classical electron models for modern physics, but rather to illuminate in some detail a specific and interesting case of the (well know) general fact that progress is often driven by a strange mixture of good and bad arguments, which hardly anybody cares to separate once progress is seen to advance in the ‘right direction’. Also, the issues connected with an inner rotational motion of the electron are hardly mentioned in the otherwise very detailed discussion of classical electron theories in the history-of-physics literature (compare [28,23]). Last but not least, the present investigation once more emphasises the importance of special-relativistic effects due to stresses, which are not necessarily connected with large velocities, at least in a phenomenological description of matter. But before giving a self-contained account, I wish to recall Pauli’s classic paper of December 1924, where he introduced his famous “classically non-describable two-valuedness”.

## 8.2 A Classically Non-Describable Two-Valuedness

### 8.2.1 Preliminaries

We begin by recalling the notion of *gyromagnetic ratio*. Consider a (not necessarily continuous) distribution of mass and charge in the context of pre-Special-Relativistic physics, like, e.g., a charged fluid or a finite number of point particles. Let  $\vec{v}(\vec{x})$  denote the corresponding velocity field with respect to an inertial frame and  $\rho_q$  and  $\rho_m$  the density distributions of electric charge and mass corresponding to the total charge  $q$  and mass  $m_0$  respectively. The total angular momentum is given by ( $\times$  denotes the antisymmetric vector product)

$$\vec{J} = \int d^3x \rho_m(\vec{x})(\vec{x} \times \vec{v}(\vec{x})). \quad (8.1)$$



The electric current distribution,  $\vec{j}(\vec{x}) := \rho_q \vec{v}(\vec{x})$ , is the source of a magnetic field which at large distances can be approximated by a sum of multipole components of increasingly rapid fall-off for large distances from the source. The lowest possible such component is the dipole. It has the slowest fall-off (namely  $1/r^3$ ) and is therefore the dominant one at large distances. (A monopole contribution is absent due to the lack of magnetic charges.) The dipole field is given by<sup>10</sup>

$$\vec{B}_{dipole}(\vec{x}) := \left(\frac{\mu_0}{4\pi}\right) \frac{3\vec{n}(\vec{n} \cdot \vec{M}) - \vec{M}}{r^3}, \quad (8.2)$$

where  $r := \|\vec{x}\|$ ,  $\vec{n} := \vec{x}/r$  and where  $\vec{M}$  denotes the magnetic dipole moment of the current distribution, which is often (we shall follow this) just called *the* magnetic moment:

$$\vec{M} := \frac{1}{2} \int d^3x \rho_q(\vec{x}) (\vec{x} \times \vec{v}(\vec{x})). \quad (8.3)$$

Note the similarity in structure to (1), except for the additional factor of 1/2 in front of (3).

The *gyromagnetic ratio* of a stationary mass and charge current-distribution,  $R_g$ , is defined to be the ratio of the moduli of  $\vec{M}$  and  $\vec{J}$ :

$$R_g := \frac{\|\vec{M}\|}{\|\vec{J}\|}. \quad (8.4)$$

We further define a dimensionless quantity  $g$ , called the *gyromagnetic factor*, by

$$R_g =: g \frac{q}{2m_0}. \quad (8.5)$$

These notions continue to make sense in non-stationary situations if  $\vec{M}$  and  $\vec{J}$  are slowly changing (compared to other timescales set by the given problem), or in (quasi) periodic situations if  $\vec{M}$  and  $\vec{J}$  are replaced by their time averages, or in mixtures of those cases where, e.g.,  $\vec{J}$  is slowly changing and  $\vec{M}$  rapidly precesses around  $\vec{J}$  (as in the case discussed below).

An important special case is given if charge and mass distributions are strictly proportional to each other, i.e.,  $\rho_q(\vec{x}) = \lambda \rho_m(\vec{x})$ , where  $\lambda$  is independent of  $\vec{x}$ . Then we have

$$R_g = \frac{q}{2m_0} \Rightarrow g = 1. \quad (8.6)$$

In particular, this would be the case if charge and mass carriers were point particles of the same charge-to-mass ratio, like  $N$  particles of one sort, where

$$\rho_q(\vec{x}) = \frac{q}{N} \sum_{i=1}^N \delta^{(3)}(\vec{x} - \vec{x}_i) \quad \text{and} \quad \rho_m(\vec{x}) = \frac{m_0}{N} \sum_{i=1}^N \delta^{(3)}(\vec{x} - \vec{x}_i). \quad (8.7)$$

After these preliminaries we now turn to Pauli's paper.

---

<sup>10</sup>We use SI units throughout so that the electric and magnetic constants  $\varepsilon_0$  and  $\mu_0$  will appear explicitly. Note that  $\varepsilon_0 \mu_0 = 1/c^2$  and that  $\mu_0 = 4\pi \cdot 10^{-7} \text{ kg} \cdot \text{m} \cdot \text{C}^{-2}$  *exactly*, where C stands for 'Coulomb', the unit of charge.

### 8.2.2 Pauli's Paper of December 1924

On December 2nd 1924, Pauli submitted a paper entitled “On the influence of the velocity dependence of the electron mass upon the Zeeman effect”<sup>11</sup> ([24], Vol. 2, pp. 201–213) to the *Zeitschrift für Physik*. In that paper he starts with the general observation that for a point particle of rest-mass  $m_0$  and charge  $q$ , moving in a bound state within a spherically symmetric potential, the velocity dependence of mass,

$$m = m_0 / \sqrt{1 - \beta^2}, \quad (8.8)$$

affects the gyromagnetic ratio. Here  $\beta := v/c$ , where  $v := \|\vec{v}\|$ . The application he aims for is the anomalous Zeeman effect for weak magnetic fields, a topic on which he had already written an earlier paper, entitled ‘On the Rules of the anomalous Zeeman Effect’<sup>12</sup> ([24], Vol. 2, pp. 151–160), in which he pointed out certain connections between the weak-field case and the theoretically simpler case of a strong magnetic field. Note that “weak” and “strong” here refers to the standard set by the inner magnetic field caused by the electrons orbital motion, so that “weak” here means that the Zeeman split is small compared to the fine-structure.

Since the charge is performing a quasi periodic motion<sup>13</sup>, its magnetic moment due to its orbital motion is given by the time average (I will denote the time average of a quantity  $X$  by  $\langle X \rangle$ )

$$\langle \vec{M} \rangle = q \langle \vec{x} \times \vec{v} \rangle / 2. \quad (8.9)$$

On the other hand, its angular momentum is given by

$$\vec{J} = m (\vec{x} \times \vec{v}) = m_0 (\vec{x} \times \vec{v}) / \sqrt{1 - \beta^2}. \quad (8.10)$$

It is constant if no external field is applied and slowly precessing around the magnetic field direction if such a field is sufficiently weak, thereby keeping a constant modulus. Hence we can write

$$\langle \vec{x} \times \vec{v} \rangle = \frac{\vec{J}}{m_0} \left\langle \sqrt{1 - \beta^2} \right\rangle, \quad (8.11)$$

where the averaging period is taken to be long compared to the orbital period of the charge, but short compared to the precession period of  $\vec{J}$  if an external magnetic field is applied. This gives

$$\frac{\|\langle \vec{M} \rangle\|}{\|\vec{J}\|} = \frac{|q|}{2m_0} \gamma, \quad (8.12)$$

where<sup>14</sup>

$$\gamma := \left\langle \sqrt{1 - \beta^2} \right\rangle. \quad (8.13)$$

---

<sup>11</sup>German original: Über den Einfluß der Geschwindigkeitsabhängigkeit der Elektronenmasse auf den Zeemaneffekt.

<sup>12</sup>German original: Über die Gesetzmäßigkeiten des anomalen Zeemaneffekts.

<sup>13</sup>Due to special-relativistic corrections, the bound orbits of a point charge in a Coulomb field are not closed. The leading order perturbation of the ellipse that one obtains in the Newtonian approximation is a prograde precession of its line of apsides.

<sup>14</sup>This is Pauli's notation. Do not confuse this  $\gamma$  with the Lorentz factor  $1/\sqrt{1 - \beta^2}$ , which nowadays is usually abbreviated by  $\gamma$ , though not in the present paper.

More specifically, Pauli applies this to the case on an electron in the Coulomb field of a nucleus. Hence  $m_0$  from now on denotes the electron mass. Its charge is  $q = -e$ , and the charge of the nucleus is  $Ze$ . Using the virial theorem, he then gives a very simple derivation of

$$\gamma = 1 + W/m_0c^2, \quad (8.14)$$

where  $W$  denotes the electron's total energy (kinetic plus potential). For the quantised one-electron problem, an explicit expression for  $W$  in terms of the azimuthal quantum number  $k$  ( $j + 1$  in modern notation, where  $j$  is the quantum number of orbital angular-momentum) and the principal quantum number  $n$  ( $n = n_r + k$ , where  $n_r$  is the radial quantum number) was known since Sommerfeld's 1916 explanation of fine structure (see, e.g., [40], p. 53, formula (17)). Hence Pauli could further write:

$$\gamma = \left\{ 1 + \frac{\alpha^2 Z^2}{\left( n - k + \sqrt{k^2 - \alpha^2 Z^2} \right)^2} \right\}^{-1/2} \approx 1 - \frac{\alpha^2 Z^2}{2n^2}, \quad (8.15)$$

where the approximation refers to small values of  $\alpha^2 Z^2$  and where  $\alpha := e^2/4\pi\epsilon_0\hbar c \approx 1/137$  is the fine-structure constant. For higher  $Z$  one obtains significant deviations from the classical value  $\gamma = 1$ . For example,  $Z = 80$  gives  $g = 0.812$ .

The relativistic correction factor  $\gamma$  affects the angular frequency<sup>15</sup> with which the magnetic moment created by the electron's orbital motion will precess in a magnetic field of strength  $B$ . This angular frequency is now given by  $\gamma\omega_0$ , where  $\omega_0$  is the Larmor (angular) frequency:

$$\omega_0 = g_e \frac{eB}{2m_0}. \quad (8.16)$$

Here we explicitly wrote down the gyromagnetic ratio,  $g_e$ , for of the electron's orbital motion even though  $g_e = 1$ , just to keep track of its appearance. The energy for the interaction of the electron with the magnetic field now likewise receives a factor of  $\gamma$ .

Pauli now applies all this to the "core model" for atoms with a single valence electron.<sup>16</sup> According to the simplest version of this model, the total angular momentum,  $\vec{J}$ , and the total magnetic moment,  $\vec{M}$ , are the vector sums of the angular and magnetic momenta of the core (indicated here by a subscript  $c$ ) and the valence electron (indicated here by a subscript  $e$ ):

$$\vec{J} = \vec{J}_c + \vec{J}_e, \quad (8.17a)$$

$$\vec{M} = \vec{M}_c + \vec{M}_e. \quad (8.17b)$$

The relations between the core's and electron's magnetic momenta on one side, and their angular momenta on the other, are of the form

$$\vec{M}_c = \frac{eg_c}{2m_0} \vec{J}_c, \quad (8.18a)$$

$$\vec{M}_e = \frac{eg_e}{2m_0} \vec{J}_e. \quad (8.18b)$$

---

<sup>15</sup>We will translate all proper frequencies in Pauli's paper into angular frequencies. Hence there are differences in factors of  $2\pi$ . This is also related to our usage of  $\hbar := h/2\pi$  rather than  $h$  (Planck's constant).

<sup>16</sup>Instead of the more modern expression "valence electron" Pauli speaks of "light electron" (German original: Lichtelektron). Sometimes the term "radiating electron" is also used (e.g., in [46]).

The point is now that  $\vec{M}$  is not a multiple of  $\vec{J}$  if  $g_e \neq g_c$ . Assuming a constant  $\vec{J}$  for the time being, this means that  $\vec{M}$  will precess around  $\vec{J}$ . Hence  $\vec{M}$  is the sum of a time independent part,  $\vec{M}_{\parallel}$ , parallel to  $\vec{J}$  and a rotating part,  $\vec{M}_{\perp}$ , perpendicular to  $\vec{J}$ . The time average of  $\vec{M}_{\perp}$  vanishes so that the effective magnetic moment is just given by  $\vec{M}_{\parallel}$ . Using (17) and (18), and resolving scalar products into sums and differences of squares,<sup>17</sup> we get

$$\begin{aligned}
 \vec{M}_{\parallel} &= \frac{\vec{J} \cdot \vec{M}}{J^2} \vec{J} \\
 &= \frac{e}{2m_0} \frac{g_e(\vec{J} \cdot \vec{J}_e) + g_c(\vec{J} \cdot \vec{J}_c)}{J^2} \vec{J} \\
 &= \frac{e}{2m_0} \frac{g_e(J^2 + J_e^2 - J_c^2) + g_c(J^2 + J_c^2 - J_e^2)}{2J^2} \vec{J} \\
 &= \frac{e}{2m_0} \left\{ g_e + (g_c - g_e) \frac{J^2 + J_c^2 - J_e^2}{2J^2} \right\} \vec{J}.
 \end{aligned} \tag{8.19}$$

Setting again  $g_e = 1$ , the expression in curly brackets gives the gyromagnetic factor of the total system with respect to the effective magnetic moment. Its quantum analog is obtained by replacing  $J^2 \rightarrow J(J+1)$  and correspondingly for  $J_c^2$  and  $J_e^2$ , which is then called the *Landé factor*<sup>18</sup>  $g_L$ . Hence

$$g_L := 1 + (g_c - 1) \frac{J(J+1) + J_c(J_c+1) - J_e(J_e+1)}{2J(J+1)}. \tag{8.20}$$

All this is still right to a good approximation if  $\vec{J}$  is not constant, but if its frequency of precession around the direction of the (homogeneous) external field is much smaller than the precession frequency of  $\vec{M}$  around  $\vec{J}$ , which is the case for sufficiently small external field strength .

Basically through the work of Landé it was known that  $g_c = 2$  fitted the observed multiplets of alkalis and also earth alkalis quite well. This value clearly had to be considered anomalous, since the magnetic moment and angular momentum of the core were due to the orbital motions of the electrons inside the core, which inevitably would lead to  $g_c = 1$ , as explained in section 8.2.1. This was a great difficulty for the core model at the time, which was generally referred to as the “magneto-mechanical anomaly”. Pauli pointed out that one could either say that the physical value of the core’s gyromagnetic factor is twice the normal value, or, alternatively, that it is obtained by adding 1 to the normal value.

These two ways of looking at the anomaly suggested two different ways to account for the relativistic correction, which should only affect that part of the magnetic moment that is due to the orbital motion of the inner electrons, that is, the ‘normal’ part of  $g_c$ . Hence Pauli considered the following two possibilities for a relativistic correction of  $g_c$ , corresponding to the two views just outlined:

$$g_c = 2 \cdot 1 \rightarrow g_c = 2 \cdot \gamma \quad \text{or} \quad g_c = 1 + 1 \rightarrow g_c = 1 + \gamma. \tag{8.21}$$

<sup>17</sup>Like, e.g.,  $\vec{J} \cdot \vec{J}_e = -\frac{1}{2}((\vec{J} - \vec{J}_e)^2 - J^2 - J_e^2) = -\frac{1}{2}(J_c^2 - J^2 - J_e^2)$ .

<sup>18</sup>For more historical background information on Landé’s impressive work on the anomalous Zeeman effect we refer to the comprehensive studies by Forman [13,12].

Then comes his final observation, that neither of these corrections are compatible with experimental results on high- $Z$  elements by Runge, Paschen and Back, which, like the low- $Z$  experiments, resulted in compatibility with (20) only if  $g_c = 2$ . In a footnote Pauli thanked Landé and Back for reassuring him that the accuracy of these measurements were about one percent. Pauli summarises his findings as follows

If one wishes to keep the hypothesis that the magneto-mechanical anomaly is also based in closed electron groups and, in particular, the  $K$  shell, then it is not sufficient to assume a doubling of the ratio of the group's magnetic moment to its angular momentum relative to its classical value. In addition, one also needs to assume a compensation of the relativistic correction. ([24], Vol. 2, p. 211)

After some further discussion, in which he stresses once more the strangeness<sup>19</sup> that lies in  $g_c = 2$ , he launches the following hypothesis, which forms the main result of his paper:

The closed electron configurations shall not contribute to the magnetic moment and angular momentum of the atom. In particular, for the alkalis, the angular momenta of, and energy changes suffered by, the atom in an external magnetic field shall be viewed exclusively as an effect of the light-electron, which is also regarded as the location [“der Sitz”] of the magneto-mechanical anomaly. The doublet structure of the alkali spectra, as well as the violation of the Larmor theorem, is, according to this viewpoint, a result of a peculiar, classically indescribable disposition of two-valuedness of the quantum-theoretic properties of the light-electron. ([24], Vol. 2, p. 213)

Note that this hypothesis replaces the atom's core as carrier of angular momentum by the valence electron. This means that (17), (18), and (20) are still valid, except that the subscript  $c$  (for “core”) is now replaced by the subscript  $s$  (for “spin”, anticipating its later interpretation), so that we now have a coupling of the electron's orbital angular momentum (subscript  $e$ ) to its intrinsic angular momentum (subscript  $s$ ). In (20), with  $g_c$  replaced by  $g_s$ , one needs to set  $g_s = 2$  in order to fit the data. But now, as long as no attempt is made to relate the intrinsic angular momentum and magnetic moment of the electron to a common origin, there is no immediate urge left to regard this value as anomalous. Also, the problem in connection with the relativistic corrections (21) now simply disappeared, since it was based on the assumption that  $\vec{J}_c$  and  $\vec{M}_c$  were due to orbital motions of inner (and hence fast) electrons, whereas in the new interpretation only  $\vec{J}_e$  and  $\vec{M}_e$  are due to orbital motion of the outer (and hence slow) valence electron.

It is understandable that this hypothesis was nevertheless felt by some to lack precisely that kind of ‘explanation’ that Pauli deliberately stayed away from: a common dynamical origin of the electron's inner angular momentum and magnetic moment. From here the ‘story of spin’ takes its course, leading to the hypothesis of the rotating electron, first conceived by Kronig and a little later by Goudsmit and Uhlenbeck, and finally to its implementation into Quantum Mechanics by Pauli [32] (“Pauli Equation” for the non-relativistic case) and Dirac [9] (fully Lorentz invariant “Dirac Equation”). Since then many myths surrounding spin built up, like that the concept of spin, and in particular

---

<sup>19</sup>For example: how can one understand the sudden doubling that the gyromagnetic factor of an outer electron must suffer when joining the core?

the value  $g = 2$ , was irreconcilable with classical (i.e. non-quantum) physics and that only the Dirac equation naturally predicted  $g = 2$ . As for the latter statement, it is well known that the principle of minimal coupling applied to the Pauli equation leads just as natural to  $g = 2$  as in case of the Dirac equation (cf. [15] and [10], p. 37). Also, the very concept of spin has as natural a home in classical physics as in quantum physics if one starts from equally general and corresponding group-theoretic considerations.<sup>20</sup>

For the rest of this contribution I wish to concentrate on the particular side aspect already outlined in the introduction. Let me repeat the question: In what sense do the actual values of the electron parameters, mass, charge, intrinsic angular-momentum, and gyromagnetic factor, resist classical modelling in the framework of Special Relativity?

### 8.3 Simple Models of the Electron

In this section we will give a self-contained summary of the basic features of simple electron models. The first model corresponds to that developed by Abraham [1], which was mentioned by Goudsmit and Uhlenbeck as already explained.<sup>21</sup> We will see that this model can only account for  $g$  factors in the interval between  $3/2$  and  $11/6$  if superluminal speeds along the equator are to be avoided. We also critically discuss the assumption made by Goudsmit and Uhlenbeck that this (i.e. Abraham's) model predicts  $g = 2$ . Since this model neglects the stresses that are necessary to prevent the charge distribution from exploding, we also discuss a second model in which such stresses (corresponding to a negative pressure in the electron's interior) are taken into account, at least in some slow-rotation approximation. This model, too, has been discussed in the literature before [7]. Here it is interesting to see that due to those stresses significantly higher values of  $g$  are possible, though not for small charges as we will also show.<sup>22</sup> Finally we discuss the restriction imposed by the condition of energy dominance, which basically says that the speed of sound of the stress-supporting material should not exceed the speed of light. This sets an upper bound on  $g$  given by  $9/4$ . Note that all these statements are made only in the realm where the slow-rotation approximation is valid. I do not know of any fully special-relativistic treatment on which generalisations of these statements could be based. In that sense, the general answer to our main question posed above is still lacking.

---

<sup>20</sup>The spaces of states in quantum and classical mechanics are Hilbert spaces and symplectic manifolds respectively. An *elementary system* is characterised in Quantum Mechanics by the requirement that the group of space-time symmetries act unitarily and irreducibly on its space of states. The corresponding requirement in Classical Mechanics is that the group action be symplectic and transitive [3]. The classification of homogeneous (with respect to the space-time symmetry group, be it the Galilei or Lorentz group) symplectic manifolds [2,22] leads then as natural to a classical concept of spin as the classification of unitary irreducible (ray-) representations leads to the quantum-mechanical spin concept. The mentioned classical structures are related to the quantum structures by various concepts of 'quantisation' like 'geometric quantisation'. Compare [49], in particular Chap.6 on elementary systems.

<sup>21</sup>Since we are mainly concerned with the spin aspects, we will ignore the differences between Abraham's and, say, Lorentz' model (rigid versus deformable), which become important as soon as translational motions are considered. We mention Abraham not for any preference for his 'rigid' model, but for the reason that he considered rotational motion explicitly. Its interaction with the translational motion was further worked out in detail by Schwarzschild in [38], but this is not important here.

<sup>22</sup>This is another example of a special-relativistic effect which has nothing to do with large velocities.

### 8.3.1 A Purely Electromagnetic Electron

Consider a homogeneous charge distribution,  $\rho$ , of total charge  $Q$  on a sphere of radius  $R$  centred at the origin (again we write  $r := \|\vec{x}\|$  and  $\vec{n} := \vec{x}/r$ ):

$$\rho(\vec{x}) = \frac{Q}{4\pi R^2} \delta(r - R). \quad (8.22)$$

For the moment we shall neglect the rest mass of the matter that sits at  $r = R$  and also the stresses it must support in order to keep the charge distribution in place. The charge is the source of the scalar potential

$$\phi(\vec{x}) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\vec{x}')}{\|\vec{x} - \vec{x}'\|} d^3x' = \frac{Q}{4\pi\epsilon_0 R} \begin{cases} 1 & \text{for } r < R, \\ R/r & \text{for } r > R, \end{cases} \quad (8.23)$$

with corresponding electric field

$$\vec{E}(\vec{x}) = \frac{Q}{4\pi\epsilon_0 R^2} \begin{cases} \vec{0} & \text{for } r < R, \\ \vec{n} & \text{for } r > R. \end{cases} \quad (8.24)$$

Let now the charge distribution rotate rigidly with constant angular velocity  $\vec{\omega}$ . This gives rise to a current density

$$\vec{j}(\vec{x}) = (\vec{\omega} \times \vec{x}) \rho(\vec{x}) = \frac{Q}{4\pi R^2} (\vec{\omega} \times \vec{x}) \delta(r - R), \quad (8.25)$$

which, in turn, is the source of a vector potential according to

$$\vec{A}(\vec{x}) = \frac{\mu_0}{4\pi} \int \frac{\vec{j}(\vec{x}')}{\|\vec{x} - \vec{x}'\|} d^3x' = \frac{\mu_0 Q}{12\pi R} \vec{\omega} \times \begin{cases} \vec{x} & \text{for } r < R, \\ \vec{x} (R/r)^3 & \text{for } r > R. \end{cases} \quad (8.26)$$

Hence, in the rotating case, there is an additional magnetic field in addition to the electric field (24):

$$\vec{B}(\vec{x}) = \frac{\mu_0}{4\pi} \begin{cases} 2\vec{M}/R^3 & \text{for } r < R, \\ (3\vec{n}(\vec{n} \cdot \vec{M}) - \vec{M})/r^3 & \text{for } r > R, \end{cases} \quad (8.27)$$

where

$$\vec{M} := \frac{1}{3}QR^2\vec{\omega}. \quad (8.28)$$

For  $r < R$  this is a constant field in  $\vec{\omega}$  direction. For  $r > R$  it is a pure dipole field (i.e. all higher multipole components vanish) with moment (28).

### Energy

The general expression for the energy of the electromagnetic field is<sup>23</sup>

$$\mathcal{E} = \int_{\mathbb{R}^3} \frac{1}{2} \left( \epsilon_0 E^2(\vec{x}) + \frac{1}{\mu_0} B^2(\vec{x}) \right) d^3x. \quad (8.29)$$

<sup>23</sup>From now on we shall denote the modulus of a vector simply by its core symbol, i.e.,  $\|\vec{E}\| = E$  etc.

For the case at hand, the electric and magnetic contributions to the energy are respectively given by

$$\mathcal{E}_e = \frac{Q^2}{8\pi\epsilon_0 R} \begin{cases} 0 & \text{from } r < R \\ 1 & \text{from } r > R \end{cases} \quad (8.30a)$$

$$\mathcal{E}_m = \frac{\mu_0}{4\pi} M^2/R^3 \begin{cases} 2/3 & \text{from } r < R \\ 1/3 & \text{from } r > R. \end{cases} \quad (8.30b)$$

The total magnetic contribution can be written as

$$\mathcal{E}_m = \frac{\mu_0}{4\pi} M^2/R^3 = \frac{1}{2} I \omega^2, \quad (8.31)$$

where

$$I := \frac{\mu_0}{18\pi} Q^2 R \quad (8.32)$$

may be called the *electromagnetic moment of inertia* [1]. It has no mechanical interpretation in terms of a rigid rotation of the electrostatic energy distribution (see below)!

The total electromagnetic energy can now be written as

$$\mathcal{E} = \mathcal{E}_e + \mathcal{E}_m = \frac{Q^2}{8\pi\epsilon_0 R} \left\{ 1 + \frac{2}{9}\beta^2 \right\}, \quad (8.33)$$

where we used  $\epsilon_0\mu_0 = 1/c^2$  and set  $\beta := R\omega/c$ . The ratio of magnetic ('kinetic') to total energy is then given by

$$\frac{\mathcal{E}_m}{\mathcal{E}} = \frac{\beta^2}{9/2 + \beta^2}, \quad (8.34)$$

which is a strictly monotonic function of  $\beta$  bounded above by 1 (as it should be). However, if we require  $\beta < 1$ , the upper bound is  $2/11$ .

### Angular Momentum

The momentum density of the electromagnetic field vanishes for  $r < R$  and is given by

$$\vec{p}(\vec{x}) = \frac{\mu_0}{16\pi^2} Q (\vec{M} \times \vec{n})/r^5 \quad (8.35)$$

for  $r > R$  ( $1/c^2$  times 'Poynting vector'). The angular-momentum density also vanishes for  $r < R$ . For  $r > R$  it is given by

$$\vec{\ell}(\vec{x}) = \vec{x} \times \vec{p}(\vec{x}) = \frac{\mu_0}{16\pi^2} Q \frac{\vec{M} - \vec{n}(\vec{n} \cdot \vec{M})}{r^4}. \quad (8.36)$$

Hence the total linear momentum vanishes, whereas the total angular momentum is given by

$$\vec{J} := \int_{r>R} \vec{\ell}(\vec{x}) d^3x = I\vec{\omega} \quad (8.37)$$

with the *same*  $I$  (moment of inertia) as in (32).



### The Gyromagnetic Factor

The gyromagnetic ratio now follows from expressions (28) for  $\vec{M}$  and (37) for  $\vec{J}$ :

$$\frac{M}{J} = \frac{6\pi R}{\mu_0 Q} =: g \frac{Q}{2m}, \quad (8.38)$$

where  $m$  denotes the total mass, which is here given by

$$m := \mathcal{E}/c^2 = \frac{\mu_0 Q^2}{8\pi R} \left\{ 1 + \frac{2}{9}\beta^2 \right\}. \quad (8.39)$$

Hence  $g$  can be solved for:

$$g = \frac{3}{2} \left\{ 1 + \frac{2}{9}\beta^2 \right\}, \quad (8.40)$$

so that

$$\frac{3}{2} < g < \frac{11}{6} \quad \text{if} \quad 0 < \beta < 1. \quad (8.41)$$

Even with that simple model we do get quite close to  $g = 2$ .

### Predicting $g = 2$ ?

It is sometimes stated that Abraham's model somehow 'predicts'  $g = 2$  (e.g., [30] p.39 or [34] p.206), though this is not at all obvious from [1]. My interpretation for how such a 'prediction' could come about can be given in terms of the present special-relativistic model.<sup>24</sup> It rests on an (inconsistent) combination of the following two observations. First, if we Lorentz transform the purely electric field (24) into constant translational motion with velocity  $w$ , we obtain a new electric and also a non-vanishing magnetic field. The integrated Poynting vector then gives the total electromagnetic momentum of the charged shell at speed  $w$ :

$$p = \frac{4}{3} \frac{m_e w}{\sqrt{1 - w^2/c^2}}, \quad (8.42)$$

where

$$m_e := \mathcal{E}_e/c^2 = \frac{\mu_0 Q^2}{8\pi R}. \quad (8.43)$$

The infamous factor  $4/3$  results from the contribution of the (unbalanced) electromagnetic stresses.<sup>25</sup> In this way one is led to assign to the electron a dynamically measurable rest-mass of  $m = \frac{4}{3}m_e$  *if one neglects the rotational energy*. Second, we may ask how fast the electron is to spin for (39) to just give  $m = \frac{4}{3}m_e$  (rest energy of the spinning

<sup>24</sup>Here we ignore Abraham's rigidity condition which would complicate the formulae without changing the argument proper. Also recall footnote 21.

<sup>25</sup>Generally speaking, the factor  $4/3$  marks the discrepancy between two definitions of 'electromagnetic mass', one through the electromagnetic momentum, the other, called  $m_e$  above, through the electrostatic energy. This discrepancy is nothing to get terribly excited about and simply a consequence of the non-conservation of the electromagnetic energy-momentum tensor, i.e.,  $\nabla_\mu T_{em}^{\mu\nu} \neq 0$ , a result of which is that the (unbalanced) electromagnetic stresses contribute to the electromagnetic momentum another third of the expression  $p = m_e w / \sqrt{1 - w^2/c^2}$  that one naively obtains from just formally transforming total energy and momentum as time and space components respectively of a four vector. Much discussion in the literature was provoked by getting confused whether this state of affairs had anything to do with Lorentz non-covariance. See, e.g., [6] for a good account and references.

electron). The immediate answer is, that this is just the case if and only if  $1 + \frac{2}{9}\beta^2 = \frac{4}{3}$ , which in view of (40) is equivalent to  $g = 2$ .

It is now obvious how this argument rests on the conflation of two different notions of mass. The factor  $4/3$  will consistently be dealt with by taking into account the stresses that balance electrostatic repulsion, not by trying to account for it in letting the electron spin fast enough.

### 8.3.2 A Side Remark on the Kinematics of Faraday Lines

In the Introduction we stressed that the emancipation of the notion of angular momentum from the usual kinematical notion of rotation in space had already begun in classical field theory. More precisely this applies to Maxwell's theory, in which the notion of a field differs from that of, say, hydrodynamics in that it is *not* thought of as being attached to a material carrier. This has consequences if we wish to apply kinematical states of motion to the field itself.

At first sight, Faraday's picture of lines of force in space suggests to view them as material entities, capable of assuming different kinematical states of motion. If so, the time-dependence of the electromagnetic field might then be interpreted as, and possibly explained by, the motions of such lines (given by some yet unknown equations of motion, of which the Maxwell equations might turn out to be some coarse grained version). That this is not possible has been stressed by Einstein in his 1920 Leiden address "Ether and the Theory of Relativity", where he writes

If one wishes to represent these lines of force as something material in the usual sense, one is tempted to interpret dynamical processes [of the em. field] as motions of these lines of force, so that each such line can be followed in time. It is, however, well known that such an interpretation leads to contradictions.

In general we have to say that it is possible to envisage extended physical objects to which the notion of motion [in space] does not apply. ([42], Vol. 7, Doc. 38, p. 315)

The reason why we mention this is that the notion of an "electromagnetic moment of inertia", introduced in (32), nicely illustrates this point. Assume that the electrostatic energy density  $\rho_e$  of the Coulomb field of charge  $Q$  corresponded to a mass density according to a local version of  $E = mc^2$ , i.e.,

$$\rho_m(\vec{x}) := \rho_e(\vec{x})/c^2 = \left(\frac{\mu_0}{32\pi^2}\right) \frac{Q^2}{r^4}. \quad (8.44)$$

If the electrostatic energy is now thought of as being attached to the somehow individuated lines of force, a moment of inertia for the shell  $R < r < R'$  would result, given by

$$I(R') = \int_{R < r < R'} \rho_m(\vec{x}) (r \sin \theta)^2 d^3x = \left(\frac{2\mu_0}{27\pi}\right) Q^2 (R' - R). \quad (8.45)$$

But this diverges as  $R' \rightarrow \infty$ , in contrast to (32), showing that we may not think of the energy distribution of the electromagnetic field as rigidly rotating in the ordinary sense.

### 8.3.3 An Electron Model with Poincaré Stresses

In this section we will modify the previous model for the electron in the following three aspects

1. The infinitesimally thin spherical shell is given a small rest-mass of constant surface density  $m_0/4\pi R^2$ .
2. Stresses in the shell are taken into account which keep the electron from exploding. They are called “Poincaré stresses” since Poincaré was the first in 1906 to discuss the dynamical need of balancing stresses [38,28].
3. The rotational velocity is small, so that  $(R\omega/c)^n$  terms are neglected for  $n \geq 2$ .

#### Poincaré Stress

The second modification needs further explanation. If we view the surface  $r = R$  as a kind of elastic membrane, there will be tangential stresses in the surface of that membrane that keep the charged membrane from exploding. In the present approximation, which keeps only linear terms in  $\omega$ , these stresses need only balance the electrostatic repulsion, which is constant over the surface  $r = R$ . In quadratic order the stresses would, in addition, need to balance the latitude dependent centrifugal forces, which we neglect here.

To calculate the surface stress that is needed to balance electrostatic repulsion we recall the expression (30a) for the electrostatic energy as function of radius  $R$ :

$$\mathcal{E}_e = \frac{Q^2}{8\pi\epsilon_0 R}. \quad (8.46)$$

Varying  $R$  gives us the differential of work that we need to supply in order to change the volume through a variation of  $R$ . Equating this to  $-pdV = -p4\pi R^2 dR$  gives the pressure inside the electron:

$$p = \left(\frac{1}{4\pi\epsilon_0}\right) \frac{Q^2}{8\pi R^4}. \quad (8.47)$$

Now, imagine the sphere  $r = R$  being cut into two hemispheres along a great circle. The pressure tries to separate these hemispheres by acting on each with a total force of strength  $p\pi R^2$  in diametrically opposite directions.<sup>26</sup> This force is distributed uniformly along the cut (the great circle), whose length is  $2\pi R$ . Hence the force per length is just  $pR/2$ . The surface stress,  $\sigma$ , (force per length) that is needed to prevent the electron from exploding is just the negative of that. Using (47), we therefore get

$$\sigma = - \left(\frac{1}{4\pi\epsilon_0}\right) \frac{Q^2}{16\pi R^3}. \quad (8.48)$$

---

<sup>26</sup>This follows immediately from the general fact that the total force along a given direction that a constant pressure exerts on a surface is given by the pressure times the area of the planar projection of that surface perpendicular to the given direction. Alternatively it may be verified directly through integrating the element of force in polar direction (i.e. perpendicular to the surface spanned by the great circle),  $dF = (p \cos \theta)(R^2 \sin \theta d\theta d\varphi)$ , over a hemisphere.

### Energy-Momentum Tensor

The energy-momentum tensor now receives a contribution that accounts for the presence of the surface stress (48) that acts tangential to the surface  $r = R$  in the local rest frame corresponding to each surface element of the rotating sphere. The four-velocity of each surface element is given by<sup>27</sup>

$$u = \partial_t + \omega \partial_\varphi, \quad (8.49)$$

which is normalised ( $g(u, u) = c^2$ ) up to terms  $\omega^2$  (which we neglect). Recall that the space-time metric of Minkowski space in spatial polar coordinates is (we use the “mostly plus” convention for the signature)

$$g = -c^2 dt \otimes dt + dr \otimes dr + r^2 d\theta \otimes d\theta + r^2 \sin^2 \theta d\varphi \otimes d\varphi. \quad (8.50)$$

The energy-momentum tensor has now three contributions, corresponding to the matter of the shell (subscript  $m$ ), the Poincaré stresses within the shell (subscript  $\sigma$ ), and the electromagnetic field (subscript  $em$ ):

$$\mathbf{T} = \mathbf{T}_m + \mathbf{T}_\sigma + \mathbf{T}_{em}. \quad (8.51a)$$

The first two comprise the shell's contribution and are given by

$$\mathbf{T}_m = \frac{m_0}{4\pi R^2} \delta(r - R) u \otimes u, \quad (8.51b)$$

$$\mathbf{T}_\sigma = - \left( \frac{1}{4\pi\epsilon_0} \right) \frac{Q^2}{16\pi R^3} \delta(r - R) \mathbf{P}. \quad (8.51c)$$

Here  $\mathbf{P}$  is the orthogonal projector onto the 2-dimensional subspace orthogonal to  $u$  and  $\partial_r$ , which is the subspace tangential to the sphere in each of its local rest frames. It can be written explicitly in terms of local orthonormal 2-legs,  $n_1$  and  $n_2$ , spanning these local 2-planes. For example, we may take  $n_1 := \frac{1}{r} \partial_\theta$  and write (since  $n_2$  must be orthogonal to  $\partial_r$  and  $\partial_\theta$ )  $n_2 = a\partial_t + b\partial_\varphi$ , where the coefficients  $a, b$  follow from  $g(u, n_2) = 0$  and normality. This gives

$$\mathbf{P} = n_1 \otimes n_1 + n_2 \otimes n_2, \quad (8.52a)$$

where

$$n_1 := \frac{1}{r} \partial_\theta, \quad (8.52b)$$

$$n_2 := c^{-2} \omega r \sin \theta \partial_t + (r \sin \theta)^{-1} \partial_\varphi. \quad (8.52c)$$

Note that  $g(n_1, n_1) = g(n_2, n_2) = 1$  and  $g(n_1, n_2) = 0$ . Equation (52a) may therefore be written in the form (again neglecting  $\omega^2$  terms)

$$\mathbf{P} = r^{-2} \partial_\theta \otimes \partial_\theta + (r \sin \theta)^{-2} \partial_\varphi \otimes \partial_\varphi + c^{-2} \omega (\partial_t \otimes \partial_\theta + \partial_\varphi \otimes \partial_t). \quad (8.53)$$

For us the crucial term will be the last one, which is off-diagonal, since it will contribute to the total angular momentum. More precisely, we will need to invoke the integral of  $\partial_t \cdot \mathbf{P} \cdot \partial_\varphi$  (the dot  $(\cdot)$  refers to the inner product with respect to the Minkowski metric) over the sphere  $r = R$ :

$$\int (\partial_t \cdot \mathbf{P} \cdot \partial_\varphi) R^2 \sin \theta d\theta d\varphi = \int c^{-2} \omega g_{tt} g_{\varphi\varphi} R^2 \sin \theta d\theta d\varphi = - \frac{8\pi}{3} \omega R^4. \quad (8.54)$$

where we used  $g_{tt} := g(\partial_t, \partial_t) = -c^2$  and  $g_{\varphi\varphi} := g(\partial_\varphi, \partial_\varphi) = R^2 \sin^2 \theta$  from (50).

<sup>27</sup>I use spacetime coordinates  $(t, r, \theta, \varphi)$  where the latter three are standard spherical polar coordinates.

I also employ the notation  $\partial_\mu := \partial/\partial x^\mu$  for the chart-induced vector fields, so that, e.g.,  $\partial_\varphi := \partial/\partial\varphi$ .

### A Note on Linear Momentum and von Laue's Theorem

The addition of the stress part has the effect that the total energy-momentum tensor is now conserved (here in the slow-rotation approximation):

$$\nabla_\mu T^{\mu\nu} = 0, \quad (8.55)$$

as one may explicitly check. Note that since we use curvilinear coordinates here we need to invoke the covariant derivative.<sup>28</sup> Indeed, writing the shell's energy momentum tensor as  $\mathbf{T}_s := \mathbf{T}_m + \mathbf{T}_\sigma$ , it is not difficult to show that  $\nabla_\mu T_s^{\mu\nu}$  is zero for  $\nu \neq r$ , and for  $\nu = r$  is given by  $p \delta(r - R)$  with  $p$  as in (47). But this clearly equals  $-\nabla_\mu T_{em}^{\mu\nu}$  since, according to Maxwell's equations, this quantity equals minus the electromagnetic force density on the charge distribution, which is obviously  $-p \delta(r - R)$ . In fact, this is precisely the interpretation that we used to determine  $p$  in the first place.

The conservation equation (55) generally ensures that total energy and total momentum form, respectively, the time- and space component of a four vector. Let us now show explicitly that  $T_\sigma$  removes the factor 4/3 in the calculation of the linear momentum when the system is boosted in ,say, the  $z$  direction. To do this we need to calculate the integral of  $\partial_z \cdot \mathbf{T}_\sigma \cdot \partial_z$  over all of space and show that it precisely cancels the corresponding integral of the electromagnetic part, i.e. the integral over  $\partial_z \cdot \mathbf{T}_{em} \cdot \partial_z$ . Noting that  $g(\partial_\theta, \partial_z) = r \sin \theta$ , we have

$$\int dV (\partial_z \cdot \mathbf{T}_\sigma \cdot \partial_z) = \int dr d\theta d\varphi (\sigma \delta(r - R) r^2 \sin^3 \theta) = \frac{8\pi}{3} \sigma R^2 = -\frac{1}{3} \mathcal{E}_e, \quad (8.56)$$

whereas the tracelessness of  $\mathbf{T}_{em}$  together with isotropy immediately imply

$$\int dV (\partial_z \cdot \mathbf{T}_{em} \cdot \partial_z) = \frac{1}{3} \int dV c^{-2} (\partial_t \cdot \mathbf{T}_{em} \cdot \partial_t) = \frac{1}{3} \mathcal{E}_e. \quad (8.57)$$

That the sum of (56) and (57) vanishes is a consequence of Laue's theorem, which basically states that the integral over all of space of the space-space components of a time-independent conserved energy-momentum tensor vanish. Here this was achieved by including stresses, which subtracted one third of the electromagnetic linear momentum.<sup>29</sup> Similarly, the stresses will also subtract from the electromagnetic angular momentum, this time even the larger portion of three quarters of it. Moreover, since the magnetic moment is the same as before, the stresses will have the tendency to increase the gyro-magnetic ratio. This we will see next in more detail

<sup>28</sup>We have  $\nabla_\mu T^{\mu\nu} = \partial_\mu T^{\mu\nu} + \Gamma_{\mu\lambda}^\mu T^{\lambda\nu} + \Gamma_{\mu\lambda}^\nu T^{\mu\lambda}$ , where  $\Gamma_{\mu\lambda}^\nu := \frac{1}{2} g^{\nu\sigma} (-\partial_\sigma g_{\mu\lambda} + \partial_\lambda g_{\sigma\mu} + \partial_\mu g_{\lambda\sigma})$ , with  $g_{\mu\nu}$  taken from (50). The  $\Gamma$ 's are most easily computed directly from the geodesic equation.

<sup>29</sup>The requirement on the stress part  $\mathbf{T}_\sigma$  to be such that the total energy and momentum derived from  $\mathbf{T}_{em} + \mathbf{T}_\sigma$  should transform as a four vector clearly still leaves much freedom in the choice of  $\mathbf{T}_\sigma$ . The choice made here is such that the total rest energy equals the electrostatic self energy. But other values for the rest energy (like, e.g., 4/3 of the electrostatic contribution) would also have been possible. In particular, the 'covariantisation through stresses' does not as such prefer any of the 'electromagnetic masses' mentioned above (footnote 25), as has also been demonstrated in an elegant and manifestly covariant fashion in [39].

### Angular Momentum

The total angular momentum represented by (51) is calculated by the general formula

$$J = -\frac{1}{c^2} \int \partial_t \cdot \mathbf{T} \cdot \partial_\varphi d^3x = J_m + J_\sigma + J_{em}. \quad (8.58a)$$

The matter part,  $J_m$ , corresponding to (51b), yields the standard expression for a mass-shell of uniform density:

$$J_m = \frac{2}{3} m_0 \omega R^2. \quad (8.58b)$$

The electromagnetic part is the same as that already calculated, since the electromagnetic field is the same. Therefore we just read off (37) and (32) that

$$J_{em} = \frac{2}{3} \cdot \frac{2}{3} m_e \omega R^2. \quad (8.58c)$$

Finally, using (54), the contribution of the stresses can also be written down:

$$J_\sigma = -\frac{1}{2} \cdot \frac{2}{3} m_e \omega R^2 = -\frac{3}{4} J_{em}. \quad (8.58d)$$

Adding the last two contributions shows that the inclusion of stresses amounts to reducing the electromagnetic contribution from the value given by (58b) to a quarter of that value:

$$J_{em} + J_\sigma = J_{em} - \frac{3}{4} J_{em} = \frac{1}{4} J_{em} \quad (8.58e)$$

In total we have

$$J = \left( m_0 + \frac{1}{6} m_e \right) \frac{2}{3} \omega R^2. \quad (8.58f)$$

To linear order in  $\omega$  the kinetic energy does not contribute to the overall mass,  $m$ , which is therefore simply given by the sum of the bare and the electrostatic mass

$$m = m_0 + m_e. \quad (8.59)$$

Using this to eliminate  $m_e$  in (58f) gives

$$J = \left( \frac{1 + 5m_0/m}{6} \right) \left( \frac{2}{3} m \omega R^2 \right). \quad (8.60)$$

### The Gyromagnetic Factor

Since the electromagnetic field is exactly as in the previous model, the magnetic moment in the present case is that given by (28). The gyromagnetic factor is defined through

$$\frac{M}{J} = g \frac{Q}{2m}, \quad (8.61)$$

which leads to

$$g = \frac{6}{1 + 5m_0/m}. \quad (8.62)$$

This allows for a range of  $g$  given by

$$1 \leq g \leq 6, \quad (8.63)$$

where  $g = 1$  corresponds to  $m = m_0$ , i.e., no electromagnetic contribution and  $g = 6$  corresponds to  $m_0 = 0$ , i.e., all mass is of electromagnetic origin. The interval (63) looks striking, given the modern experimental values for the electron and the proton:

$$g_{\text{electron}} = 2.0023193043622 \quad \text{and} \quad g_{\text{proton}} = 5.585694713. \quad (8.64)$$

However, we have not yet discussed the restrictions imposed by our slow-rotation assumption. This we shall do next.

### Restrictions by Slow Rotation

Our model depends on the four independent parameters,  $P = (m_0, Q, R, \omega)$ . On the other hand, there are four independent physical observables,  $O = (m, Q, g, J)$  ( $M$  is dependent through (61)). Our model provides us with a functional dependence expressing the observables as functions of the parameters:  $O = O(P)$ . Since  $Q$  is already an observable, it remains to display  $m, g, J$  in terms of the parameters:

$$m(m_0, Q, R) = m_0 + \frac{\mu_0 Q^2}{8\pi R} =: m_0 + m_e(Q, R), \quad (8.65a)$$

$$g(m_0, Q, R) = \frac{6}{1 + 5m_0/m(m_0, Q, R)}, \quad (8.65b)$$

$$J(m_0, Q, R, \omega) = \left(m_0 + \frac{1}{6}m_e(Q, R)\right) \frac{2}{3}\omega R^2. \quad (8.65c)$$

These relations can be inverted so as to allow the calculation of the values of the parameters from the values of the observables. If we choose to display  $\beta := R\omega/c$  rather than  $\omega$ , this gives

$$m_0(m, g) = m \frac{6-g}{5g}, \quad (8.66a)$$

$$m_e(m, g) = m - m_0 = m \frac{6(g-1)}{5g}, \quad (8.66b)$$

$$R(m, Q, g) = \frac{\mu_0 Q^2}{8\pi m_e} = \frac{\mu_0 Q^2}{8\pi m} \frac{5g}{6(g-1)} \quad (8.66c)$$

$$\beta(J, Q, g) = 2J \left[ \frac{Q^2}{4\pi\epsilon_0 c} \right]^{-1} \frac{9(g-1)}{5}, \quad (8.66d)$$

where the last equation (66d) follows from (65c) using (66a–66c). It is of particular interest to us since it allows to easily express the slow-rotation assumption  $\beta \ll 1$ . For this it will be convenient to measure  $Q$  in units of the elementary charge  $e$  and  $J$  in units of  $\hbar/2$ . Hence we write

$$Q = n_Q e \quad \text{and} \quad 2J = n_J \hbar. \quad (8.67)$$

Then, using that the fine-structure constant in SI units reads  $\alpha = e^2/(4\pi\epsilon_0 c\hbar) \approx 1/137$ , we get

$$\beta = \frac{n_J}{n_Q^2} \alpha^{-1} \frac{9(g-1)}{5}. \quad (8.68)$$

This nicely shows that the slow-rotation approximation constrains the given combination of angular momentum, charge, and gyromagnetic factor. In particular, any gyromagnetic factor up to  $g = 6$  can be so obtained, given that the charge is sufficiently large. If we set  $g = 2$  and  $n_J = 1$  (corresponding to the electron's values), we get

$$n_Q \gg \sqrt{n_J(g-1)247} \approx 16. \quad (8.69)$$

This means that indeed we cannot cover the electrons values with the present model while keeping the slow-rotation approximation, though this model seems to be able to accommodate values of  $g$  up to six if the charge is sufficiently high. However, we did not check whether the assumption that the matter of the shell provided the stabilising stresses is in any way violating general conditions to be imposed on any energy-momentum tensor. This we shall do next.

### Restrictions by Energy Dominance

Energy dominance essentially requires the velocity of sound in the stress-supporting material to be superluminal. It is conceivable that for certain values of the physical quantities  $(m, Q, g, J)$  the stresses would become unphysically high. To check that, at least for the condition of energy dominance, we first note from (51c) and (43) that the stress part of the energy-momentum tensor can be written in the form

$$\mathbf{T}_\sigma = -\frac{1}{2} \frac{m_e}{4\pi R^2} c^2 \delta(r-R) \mathbf{P}. \quad (8.70)$$

Hence the ratio between the stress within the shell (in any direction given by the unit spacelike vector  $n$  tangent to the shell, so that  $n \cdot \mathbf{P} \cdot n = 1$ ) and its energy density, as measured by a locally co-rotating observer, is given by

$$\left| \frac{n \cdot \mathbf{T} \cdot n}{u \cdot \mathbf{T} \cdot u} \right| = \frac{m_e}{2m_0} = \frac{3(g-1)}{6-g}, \quad (8.71)$$

where we used (66a) and (66b) in the last step. The condition of energy dominance now requires this quantity to be bounded above by 1, so that

$$\frac{3(g-1)}{6-g} \leq 1 \iff g \leq \frac{9}{4}. \quad (8.72)$$

Interestingly this depends on  $g$  only. Hence we get, after all, an upper bound for  $g$ , though from the condition of energy dominance, i.e. a subluminal speed of sound in the shell material, and not from the condition of a subluminal rotational speed.

### The Size of the Electron

What is the size of the electron? According to (66c), its radius comes out to be

$$R = \frac{1}{4\pi\epsilon_0 c^2} \frac{e^2}{2m} \frac{5}{3}, \quad (8.73)$$

where we set  $Q = -e$  and  $g = 2$ . On the other hand, in Quantum Mechanics, the Compton wavelength of the electron is

$$\lambda = \frac{2\pi\hbar}{mc}, \quad (8.74)$$



so that their quotient is just

$$\frac{R}{\lambda} = \frac{5}{6} \frac{\alpha}{2\pi} \approx 2 \cdot 10^{-3}. \quad (8.75)$$

This might first look as if the classical electron is really small, at least compared to its Compton wavelength. However, in absolute terms we have (fm stands for the length scale “Fermi”)

$$R \approx 2 \cdot 10^{-15} \text{ m} = 2 \text{ fm}, \quad (8.76)$$

which is very large compared to the scale of  $10^{-3}$  fm at which modern high-energy experiments have probed the electron’s structure, so far without any indication for substructures. At that scale the model discussed here is certainly not capable of producing any reasonable values for the electron parameters, since the electrostatic mass (and hence the total mass, if we assume the weak energy-condition,  $m_0 > 0$ , for the shell matter) comes out much too large and the angular momentum much too small (assuming  $\beta < 1$ ).

One might ask whether the inclusion of gravity will substantially change the situation. For example, one would expect the gravitational binding to reduce the electrostatic self-energy. An obvious and answerable questions is whether the electron could be a Black Hole? What is particularly intriguing about spinning and charged Black Holes in General Relativity is that their gyromagnetic factor is  $g = 2$ , always and exactly!<sup>30</sup> For a mass  $M$  of about  $10^{-30}$  kg to be a Black Hole it must be confined to a region smaller than the Schwarzschild radius  $R_s = 2GM/c^2 \approx 10^{-57}$  m, which is almost 40 orders of magnitude below the scale to which the electron structure has been probed and found featureless. Hence, leaving alone Quantum Theory, it is certainly a vast speculation to presume the electron to be a Black Hole. But would it also be inconsistent from the point of view of General Relativity? The Kerr-Newman family of solutions for the Einstein-Maxwell equations allow any parameter values for mass (except that it must be positive), charge, and angular momentum. As already stated,  $g = 2$  automatically. Hence there is also a solution whose parameter values are those of the electron. However, only for certain restricted ranges of parameter values do these solutions represent Black Holes, that is, possess event horizons that cover the interior singularity; otherwise they contain naked singularities.

More precisely, one measures the mass  $M$ , angular momentum per unit mass  $A$ , and charge  $Q$  of a Kerr-Newman solution in geometric units, so that each of these quantities acquires the dimension of length. If we denote these quantities in geometric units by the corresponding lower case letters,  $m$ ,  $a$ , and  $q$  respectively, we have

$$m = M \frac{G}{c^2}, \quad (8.77a)$$

$$a = \frac{A}{c}, \quad (8.77b)$$

$$q = Q \sqrt{\frac{\mu_0}{4\pi} \frac{G}{c^2}}. \quad (8.77c)$$

The necessary and sufficient condition for an event horizon to exist is now given by

$$\left(\frac{a}{m}\right)^2 + \left(\frac{q}{m}\right)^2 \leq 1. \quad (8.78)$$

---

<sup>30</sup>It is known that  $g = 2$  is already a preferred value in special-relativistic electrodynamics [4], a fact on which modern precision measurements of  $g - 2$  rest. See [34] and [16] for instructive discussions as to what makes  $g = 2$  also a special value in General Relativity.

The relevant quantities to look at are therefore the dimensionless ratios<sup>31</sup>

$$\frac{a}{m} = \frac{A}{M} \cdot \frac{c}{G} \approx \frac{A[\text{m}^2 \cdot \text{s}^{-1}]}{M[\text{kg}]} \cdot 5.5 \cdot 10^{18}, \quad (8.79a)$$

$$\frac{q}{m} = \frac{Q}{M} \cdot \sqrt{\frac{\mu_0}{4\pi}} \frac{c^2}{G} \approx \frac{Q[\text{C}]}{M[\text{kg}]} \cdot 10^{10}. \quad (8.79b)$$

Now, if we insert the parameter values for the electron<sup>32</sup> (we take for  $Q$  the modulus  $e$  of the electron charge) we arrive at the preposterous values

$$\left. \frac{a}{m} \right|_{\text{electron}} \approx (5 \cdot 10^{25}) (5.5 \cdot 10^{18}) \approx 2.5 \cdot 10^{44}, \quad (8.80a)$$

$$\left. \frac{q}{m} \right|_{\text{electron}} \approx (1.6 \cdot 10^{11}) \cdot 10^{10} \approx 1.6 \cdot 10^{21}, \quad (8.80b)$$

so that we are indeed very far from a Black Hole. Classically one would reject the solution for the reason of having a naked singularity. But note that this does not exclude the possibility that this exterior solution is valid up to some finite radius, and is then continued by another solution that takes into account matter sources other than just the electromagnetic field.<sup>33</sup>

## 8.4 Summary

Understanding the generation of new ideas and the mechanisms that led to their acceptance is a common central concern of historians of science, philosophers of science, and the working scientists themselves. The latter might even foster the hope that important lessons can be learnt for the future. In any case, it seems to me that from all perspectives it is equally natural to ask whether a specific argument is actually true or just put forward for persuasive reasons.

Within the history of Quantum Mechanics the history of spin is, in my opinion, of particular interest, since it marks the first instance where a genuine quantum degree of freedom without a classically corresponding one were postulated to exist. If this were the general situation, our understanding of a quantum theory as the quantisation of a classical theory cannot be fundamentally correct.<sup>34</sup> On the other hand, modern theories

<sup>31</sup>We write  $P[X]$  to denote the number that gives the physical quantity  $P$  in units of  $X$ .

<sup>32</sup>We have  $A = S/M$  with  $S = \frac{1}{2}\hbar$  (modulus of electron spin) and use the approximate values  $\hbar[\text{J} \cdot \text{s}] \approx 10^{-34}$ ,  $M[\text{kg}] = 10^{-30}$ , and  $Q[\text{C}] = 1.6 \cdot 10^{-19}$ .

<sup>33</sup>Even in mesoscopic situations  $a < m$  means a very small angular momentum indeed. Recall that in Newtonian approximation the angular momentum of a homogeneous massive ball of radius  $R$  is  $2MR^2\omega/5$ , so that  $a/m \leq 1$  translates to the following inequality for the spin period  $T = 2\pi/\omega$ :

$$T \geq \frac{4\pi}{5} \frac{R}{c} \frac{R}{m} \approx \frac{R^2[\text{m}]}{M[\text{kg}]} \cdot 10^{19} \text{ sec}, \quad (8.81)$$

which for a ball of radius one meter and mass  $10^3$  kilogrammes sets an upper bound for  $T$  of  $3 \cdot 10^8$  years! In fact, (81) is violated by all planets in our solar system.

<sup>34</sup>I take this to be an important and very fundamental point. Perhaps with the exception of Axiomatic Local Quantum Field Theory, any quantum theory is in some sense the quantisation of a classical theory. Modern mathematical theories of 'quantisation' understand that term as 'deformation' (in a precise mathematical sense) of the algebra of observables over *classical* phase space; cf. [48].

of quantisation can explain the quantum theory of a spinning particle as the result of a quantisation applied to some classical theory, in which the notion of spin is already present.<sup>35</sup> Hence, from a modern perspective, it is simply not true that spin has no classical counterpart. That verdict (that is has no classical counterpart), which is still often heard and/or read<sup>36</sup>, is based on a narrow concept of ‘classical system’, which has been overcome in modern formulations, as was already mentioned in footnote 20 to which I refer at this point. From that point of view, spin is no less natural in classical physics than in Quantum Theory, which has now become the standard attitude in good textbooks on analytical mechanics, e.g. [41,22] as well as in attempts to formulate theories of quantisation [48,49].

In the present contribution I concentrated on another aspect, namely whether it is actually true that classical models for the electron (as they were already, or could have been, established around 1925) are not capable to account for the actual values of the four electron parameters: mass, charge, angular momentum, and the gyromagnetic factor. This criticism was put forward from the very beginning (Lorentz) and was often repeated thereafter. It turns out that this argument is not as clear cut as usually implied. In particular,  $g = 2$  is by no means incompatible with classical physics. Unfortunately, explicit calculations seem to have been carried out only in a simplifying slow-rotation approximation, in which the Poincaré stresses may be taken uniform over the charged shell. In the regime of validity of this approximation  $g = 2$  is attainable, but not for small charges. I do not think it is known whether and, if so, how an exact treatment improves on the situation. In that sense, the answer to the question posed above is not known. An exact treatment would have to account for the centrifugal forces that act on the rotating shell in a latitude dependent way. As a result, the Poincaré stresses cannot retain the simple (constant) form as in (51c) but must now also be latitude dependent. In particular, they must be equal in sign but larger in magnitude than given in (48) since now they need in addition to balance the outward pushing centrifugal forces. On one hand, this suggests that their effect is a still further reduction of angular momentum for fixed magnetic moment, resulting in still larger values for  $g$ . On the other hand, fast rotational velocities result in an increase of the inertial mass according to (8) and hence an increase of angular momentum, though by the same token also an increase in the centrifugal force and hence an increase in stress. How the account of these different effects finally turns out to be is unclear (to me) without a detailed calculation.<sup>37</sup> It would be of interest to return to this issue in the future.

**Acknowledgements** I thank one of the anonymous referees for suggesting more care in calling the work of Goudsmit’s and Uhlenbeck’s ‘independent’ of the earlier one by Kronig (cf. footnote 1), as done in an earlier version, and also for pointing out reference [8].

---

<sup>35</sup>Namely in the sense that it has a corresponding classical state space given by a two-sphere, which is a symplectic manifold. However, this state space is not the phase space (i.e. cotangent bundle) over some space of classical configurations, so that one might feel hesitant to call it a classical *degree of freedom*.

<sup>36</sup>Even in critical historical accounts, e.g.: “Indeed, there were unexpected results from quantum theory such as the fact that the electron has a fourth degree of freedom, namely, a spin which has no counterpart in a classical theory” ([28], p. 319).

<sup>37</sup>In that respect the corresponding statements made in Sect. 4.7.1 of [37] seem to me premature.

## References

- [1] Max Abraham. Prinzipien der Dynamik des Elektrons. *Annalen der Physik*, 315(1): 105–179, 1902.
- [2] Richard Arens. Classical Lorentz invariant particles. *Journal of Mathematical Physics*, 12(12): 2415–2422, 1971.
- [3] Henri Bacry. Space-time and degrees of freedom of the elementary particle. *Communications in Mathematical Physics*, 5(2): 97–105, 1967.
- [4] Valentine Bargmann, Louis Michel, and Valentine L. Telegdi. Precession of the polarization of particles moving in a homogeneous electromagnetic field. *Physical Review Letters*, 2(10): 435–436, 1959.
- [5] Max Born. *Atomic Physics*. Dover Publications, Inc., New York, 1989. Unabridged and unaltered republication of the eighth edition (1969) of the work first published in 1935 by Blackie & Son Ltd., Glasgow.
- [6] Ignacio Campos and José Luis Jiménez. Comment on the 4/3 problem in the electromagnetic mass and the Boyer-Rohrlich controversy. *Physical Review D*, 33(2): 607–610, 1986.
- [7] Jeffrey M. Cohen and Errol Mustafa. Can classical physics give  $g$ -factors  $> 1$ ? *Physics Letters A*, 115(6): 265–267, 1986.
- [8] Hans Dehmelt. New continuous Stern-Gerlach Effect and a Hint of the Elementary Particle. *Zeitschrift für Physik D*, 10(5): 127–134, 1988.
- [9] Paul A.M. Dirac. The quantum theory of the electron. *Proceedings of the Royal Society of London. Series A*, 117(778): 610–624, 1928.
- [10] Richard Feynman. *Quantum Electrodynamics. A Lecture Note and Reprint Volume. Frontiers in Physics*. W.A. Benjamin, Inc., New York, 1961.
- [11] Markus Fierz and Victor F. Weisskopf, editors. *Theoretical Physics in the Twentieth Century. A Memorial Volume to Wolfgang Pauli*. Interscience Publishers Inc., New York, 1960.
- [12] Paul Forman. The doublet riddle and atomic physics circa 1924. *Isis*, 59(2): 156–174, 1968.
- [13] Paul Forman. Alfred Landé and the anomalous Zeeman effect, 1919–1921. *Historical Studies in the Physical Sciences*, 2: 153–261, 1970.
- [14] Jacov Ilich Frenkel. Die Elektrodynamik des rotierenden Elektrons. *Zeitschrift für Physik*, 37(4–5): 243–262, 1926.
- [15] Alberto Galindo and Carlos Sanchez Del Rio. Intrinsic magnetic moment as a nonrelativistic phenomenon. *American Journal of Physics*, 29(9): 582–584, 1961.

- [16] David Garfinkle and Jennie Traschen. Gyromagnetic ratio of a black hole. *Physical Review D*, 42(2): 419–423, 1990.
- [17] Domenico Giulini. Algebraic and geometric structures in special relativity. In Claus Lämmerzahl and Jürgen Ehlers, editors, *Special Relativity: Will it Survive the Next 101 Years?*, volume 702 of *Lecture Notes in Physics*, pages 45–111. Springer Verlag, Berlin, 2006. Online available at [arxiv.org/pdf/mathph/0602018](http://arxiv.org/pdf/mathph/0602018).
- [18] Samuel A. Goudsmit. The discovery of the electron spin. Online available at [www.lorentz.leidenuniv.nl/history/spin/goudsmit.html](http://www.lorentz.leidenuniv.nl/history/spin/goudsmit.html). Concluding lecture given at the occasion of the golden jubilee meeting of the Dutch Physical Society in April 1971.
- [19] Samuel A. Goudsmit. It might as well be spin. *Physics Today*, 29(6): 40–43, 1976.
- [20] Samuel A. Goudsmit and George E. Uhlenbeck. Ersetzung der Hypothese vom unmechanischen Zwang durch eine Forderung bezüglich des inneren Verhaltens jedes einzelnen Elektrons. *Die Naturwissenschaften*, 47: 953–954, 1925.
- [21] Samuel A. Goudsmit and George E. Uhlenbeck. Spinning electrons and the structure of spectra. *Nature*, 117: 264–265, 1926.
- [22] Victor Guillemin and Shlomo Sternberg. *Symplectic Techniques in Physics*. Cambridge University Press, Cambridge, 1990. Corrected reprint.
- [23] Michel Janssen and Matthew Mecklenburg. From classical to relativistic mechanics: Electromagnetic models of the electron. *Boston Studies in the Philosophy of Science*, 251: 65–134, 2006.
- [24] Ralph Kronig and Victor F. Weisskopf, editors. *Collected Scientific Papers by Wolfgang Pauli, Vols. 1–2*. Interscience Publishers, a division of John Wiley & Sons, Inc., New York, 1964.
- [25] Ralph de Laer Kronig. The magnetic moment of the electron. *Proceedings of the National Academy of Sciences of the United States of America*, 12(5): 328–330, 1926.
- [26] Ralph de Laer Kronig. Spinning electrons and the structure of spectra (letter to the editor). *Nature*, 117: 550, 1926.
- [27] Karl von Meyenn, editor. *Wolfgang Pauli: Scientific Correspondence with Bohr, Einstein, Heisenberg, a.O.*, Vol. I–IV, volume 2, 6, 11, 14, 15, 17, 18 of *Sources in the History of Mathematics and Physical Sciences*. Springer Verlag, Heidelberg and New York, 1979–2005.
- [28] Arthur I. Miller. A study of Henri Poincaré’s *Sur la Dynamique de l’ Electron*. *Archive for History of Exact Sciences*, 10(3–5): 207–328, 1973.
- [29] Neville F. Mott. The scattering of fast electrons by atomic nuclei. *Proceedings of the Royal Society of London, Series A*, 124(794): 425–442, 1929.

- [30] Abraham Pais. George Uhlenbeck and the discovery of electron spin. *Physics Today*, 42(12): 34–40, 1989.
- [31] Wolfgang Pauli. Exclusion principle and quantum mechanics. Online available via <http://nobelprize.org>. Nobel Lecture delivered on December 13th 1946 for the 1945 Nobel Prize in Physics.
- [32] Wolfgang Pauli. Zur Quantenmechanik des magnetischen Elektrons. *Zeitschrift für Physik*, 43(9–10): 601–623, 1927.
- [33] Wolfgang Pauli. *Die allgemeinen Prinzipien der Wellenmechanik*. Springer Verlag, Berlin, 1990. Newly edited and annotated by Norbert Straumann.
- [34] Herbert Pfister and Markus King. The gyromagnetic factor in electrodynamics, quantum theory and general relativity. *Classical and Quantum Gravity*, 20: 205–213, 2003.
- [35] Henri Poincaré. Sur la dynamique de l'électron. *Rediconti del Circolo Matematico di Palermo*, 21: 129–176, 1906. Submitted July 1905, printed 14th December 1905.
- [36] Robert Rossmanith. Polarized antiprotons with the spin splitter. *American Institute of Physics Conference Proceedings*, 176(1): 271–276, 1988. Online version (with coauthors) available at [accelconf.web.cern.ch/accelconf/e88/PDF/EPAC1988-0848.PDF](http://accelconf.web.cern.ch/accelconf/e88/PDF/EPAC1988-0848.PDF).
- [37] Marcus Schulte. Die Bedeutung des Spinbegriffs. Available online at <http://deposit.ddb.de/cgi-bin/dokserv?idn=960517863>. Dissertation at FB 14 of the University of Dortmund, December 1999.
- [38] Karl Schwarzschild. Zur Elektrodynamik. III. Über die Bewegung des Elektrons. *Königliche Gesellschaft der Wissenschaften zu Göttingen. Mathematisch Physikalische Klasse. Nachrichten*, 245–278, 1903.
- [39] Julian Schwinger. Electromagnetic mass revisited. *Foundations of Physics*, 13(3): 373–383, 1983.
- [40] Arnold Sommerfeld. Zur Quantentheorie der Spektrallinien. *Annalen der Physik*, 51(17): 194, 1916.
- [41] Jean-Marie Souriau. *Structure of Dynamical Systems: A Symplectic View of Physics*, volume 149 of *Progress in Mathematics*. Birkhäuser Verlag, Boston, 1997. Translation by C.H. Cushman de Vries of the 1970 French original.
- [42] John Stachel et al., editors. *The Collected Papers of Albert Einstein, Vols. 1–9*. Princeton University Press, Princeton, New Jersey, 1987–2005.
- [43] Igor Mikhailovich Ternov and Vladimir A. Bordovitsyn. Modern interpretation of J. I. Frenkel's classical spin theory. *Soviet Physics Uspekhi*, 23(10): 679–683, 1980.
- [44] Llewellyn Hilleth Thomas. The motion of the spinning electron. *Nature*, 117: 514, 1926.

- [45] Llewellyn Hilleth Thomas. The kinematics of an electron with an axis. *Philosophical Magazine*, 3: 1–22, 1927.
- [46] Sin-itiro Tomonaga. *The Story of Spin*. The University of Chicago Press, Chicago, 1997. Translation by Takeshi Oka of the 1974 Japanese original.
- [47] George E. Uhlenbeck. Personal reminiscences. *Physics Today*, 29(6): 43–48, 1976.
- [48] Stefan Waldmann. *Poisson-Geometrie und Deformationsquantisierung. Eine Einführung*. Springer Verlag, Berlin, 2007.
- [49] Nicholas Woodhouse. *Geometric Quantization*. Clarendon Press, Oxford, second edition, 1991.

# 9 First Steps (and Stumbles) of Bose-Einstein Condensation

DANIELA MONALDI

## Introduction

In 1924, Einstein predicted the occurrence of condensation in an ideal gas. He published the prediction at the beginning of 1925, in the second of his papers on the application of Bose's statistical method to a gas of particles. The theoretical physicist Chen Ning Yang called this prediction "a most daring and insightful extrapolation which has only now been brilliantly experimentally confirmed."<sup>1</sup> Yang was referring to the experimental observation of the phenomenon known as Bose-Einstein condensation in dilute gases, which was achieved in 1995 and was awarded the Nobel Prize in physics in 2001. The Bose-Einstein condensation produced and observed in 1995 in real gases, in fact, is universally identified with the process predicted by Einstein seventy years earlier.

There are two kinds of historical narratives in which Einstein's prediction appears. When the history of Bose-Einstein condensation is outlined, it is often said that Einstein predicted a new kind of phase transition. For example, a text of the Royal Swedish Academy of Sciences reads,

Einstein noted that if the number of particles is conserved even totally non-interacting particles will undergo a phase transition at low enough temperatures. This transition is termed Bose-Einstein condensation (BEC).<sup>2</sup>

Einstein's prediction is cast against the backdrop of a supposedly familiar notion of phase transitions, while its novelty of being caused solely by quantum statistics and not by intermolecular interactions is highlighted. It is implicitly suggested that Einstein relied on a pre-existing theory of phase transitions to make the prediction.

Yet, when the history of phase transitions is recalled, Bose-Einstein condensation is listed as one of a group of phenomena, along with ordinary gas-liquid transitions, ferromagnetism, the He-I to He-II transition, and superconductivity, from which a general idea of phase transition gradually emerged, making it possible to attempt formulating an encompassing classification, common theoretical concepts, and a unified theoretical picture.

My main point will be that the history of Bose-Einstein condensation is more complex than the script about the final verification of an "insightful" theoretical prediction implies. In particular, the history of Bose-Einstein condensation cannot be decoupled from

---

<sup>1</sup>Chen Ning Yang, "Remarks About Some Developments in Statistical Mechanics", HFPN, Number 06, March 15, 1996, available at <http://chris.kias.re.kr/yang.htm>.

<sup>2</sup>Royal Swedish Academy of Sciences, "Advanced information on the Nobel Prize in Physics 2001", [http://nobelprize.org/nobel\\_prizes/physics/laureates/2001/phyadv.pdf](http://nobelprize.org/nobel_prizes/physics/laureates/2001/phyadv.pdf).



the history of phase transitions. I shall concentrate on an episode to which neither of the two narratives I sketched above pays much attention. We find this episode recounted, instead, when the focus is on the anecdotic or the biographical; it is typically characterized as a detour that “delayed the general acceptance of the Bose-Einstein condensation for 10 years”.<sup>3</sup> For over a decade Einstein’s prediction was “not taken terribly seriously even by Einstein himself”, and “rather got the reputation of having only a purely imaginary existence,” until it was “resurrected” by Fritz London in 1938 in connection with a possible clarification of the “lambda transition” in liquid He.<sup>4</sup> Yet, this very detour might offer an insight on how the history of Bose-Einstein condensation and the history of phase transitions are interrelated.

There appear to be two reasons for the long neglect of Einstein’s prediction. The first is that in 1927 George E. Uhlenbeck severely questioned Einstein’s argument. Uhlenbeck’s criticism persuaded even Einstein that the prediction was mistaken. The second reason is that the predicted phenomenon “appeared to be devoid of any practical significance[.]”<sup>5</sup> Einstein himself had admitted that, although the densities of real gases such as helium and hydrogen could reach values not too far from the saturation values that would mark the onset of condensation in the corresponding ideal gases, the effects of quantum degeneracy would be obscured by molecular interactions.<sup>6</sup> In the following decades, although the onset of Bose-Einstein condensation was not in itself considered to be beyond the reach of experiment, the densities required were so high and the temperatures so low that, as Schrödinger wrote in 1946,

the van der Waals corrections are bound to coalesce with the possible effects of degeneration, and there is little prospect of ever being able to separate the two kinds of effect.<sup>7</sup>

The conviction that Bose-Einstein condensation could never be observed in real gases was abandoned only in the late 1970s, when the suggestion that spin-polarized hydrogen would remain gaseous down to zero temperature, together with tremendous advances in the technology of ultracold temperatures, triggered the first efforts toward an experimental realization of the phenomenon.

Uhlenbeck, however, withdrew his objection in 1937, thus clearing the way for London’s resurrection of Bose-Einstein condensation as a possible theoretical model for the underlying mechanism of the lambda transition in liquid helium. As I shall try to show, this alleged resurrection was in fact a new formulation of the condensation prediction based on a new understanding of phase transitions.

---

<sup>3</sup>E. G. D. Cohen, “George E. Uhlenbeck and statistical mechanics”, *American Journal of Physics*, 58 (1990), 619–625, on 619. See also A. Pais, “Einstein and the quantum theory”, *Reviews of Modern Physics*, 51 (1979), 863–914, on 897; G. E. Uhlenbeck, “Some Reminiscences About Einstein’s Visit to Leiden”, in H. Woolf, ed., *Some Strangeness in the Proportion. A Centennial Symposium to Celebrate the Achievements of Albert Einstein* (Reading, MA: Addison-Wesley Publishing Company, 1980), 524–525.

<sup>4</sup>Eric A. Cornell and Carl E. Wiemann, “Bose-Einstein condensation in a Dilute Gas; The First 70 Years and Some Recent Experiments”, *Les Prix Nobel. The Nobel Prizes 2001*, T. Frängsmyr, ed. (Stockholm: Nobel Foundation, 2002), 78–108, on 78; F. London, “The  $\lambda$ -phenomenon of Liquid Helium and the Bose-Einstein Degeneracy”, *Nature*, 141, 643–644, on 644.

<sup>5</sup>F. London, “On the Bose-Einstein condensation”, *Physical Review*, 54 (1938), 947–954, on 947.

<sup>6</sup>Einstein, “Quantentheorie des einatomigen idealen Gases. Zweite Abhandlung”, *Berliner Berichte* (1925), 3–14, on 11–12.

<sup>7</sup>E. Schrödinger, *Statistical Thermodynamics* (Cambridge, 1967), on 54.

## Einstein's Argument

Einstein's 1925 prediction was as follows:

In the theory of the ideal gas, it seems a self-evident requirement that volume and temperature of a quantity of gas can be given arbitrarily. The theory determines then the energy or the pressure of the gas. But the study of the equation of state contained in equations (18), (19), (20), (21) shows that if the number of molecules  $n$  and the temperature  $T$  are given, the volume cannot be made arbitrarily small. [...] *But then, what happens if I let the density of the substance,  $\frac{n}{V}$ , increase further at this temperature (for example, by isothermal compression)?*

*I assert that in this case a number of molecules, a number increasing with the total density, passes into the first quantum state (state without kinetic energy), while the remaining molecules distribute themselves according to the parameter value  $\lambda = 1$ . Thus, the assertion means that *there occurs something similar to* when isothermally compressing a vapour above the saturation volume. A separation takes place; a part "condenses", the rest remains a "saturated ideal gas" ( $A = 0, \lambda = 1$ ).<sup>8</sup>*

In this text, the expression "I assert [*Ich behaupte*]" makes a contrast with the language of the previous sentences, "The study of the equations shows... It follows from..." Einstein wanted to tell us that his *Behauptung* was no deduction from the preceding theory. In fact, he formulated it as a way out from what would have otherwise been a serious limitation of the theory. And he drew it only on the basis of a physical model, the model of a vapour at the saturation volume, without having a formal analogy to go with it.

Einstein had derived for the total number of particles of his ideal gas the expression,

$$n = \sum_S \frac{1}{\frac{1}{\lambda} e^{\frac{E_S}{kT}} - 1} \quad (1)$$

---

<sup>8</sup>A. Einstein, "Quantentheorie. Zweite Abhandlung" (note 6), on 3-4, emphasis added. The equations referred to in the quotation are,

$$n = \sum_{\sigma} \frac{1}{e^{\alpha^S} - 1} \quad (18)$$

$$\bar{E} = \frac{3}{2} pV = c \sum_{\sigma} \frac{s^{\frac{2}{3}}}{e^{\alpha^S} - 1} \quad (19)$$

$$\alpha^S = A + \frac{cs^{\frac{2}{3}}}{xT} \quad (20)$$

$$c = \frac{E^S}{s^{\frac{2}{3}}} = \frac{h}{2m} \left( \frac{4}{3} \pi V \right)^{-\frac{2}{3}} \quad (21)$$

where  $A$  is defined by equation (16),  $e^A = \pi^{\frac{3}{2}} h^{-3} \frac{V}{n} (2m x T)^{\frac{3}{2}}$ . Einstein defined the parameter  $\lambda$  by the statement, "...the quantity  $e^{-A}$ , which we want to indicate by  $\lambda$ ..." . Einstein, "Quantentheorie des einatomigen idealen Gases", *Berliner Berichte* (1924), 261-267, on 265-266. Today, the letter  $\lambda$  is commonly used for another quantity, *the thermal de Broglie wavelength* of the gas,  $\lambda_{dB} \equiv \frac{h}{\sqrt{2\pi m k T}}$ , which is related to Einstein's parameter by  $\lambda = \frac{n}{V} \lambda_{dB}^3$ .

and had identified the parameter  $\lambda$  as “*ein Maß für die ‘Entartung’ des Gases.*”<sup>9</sup> In order to examine the dependence of the number of particles on the volume and on the temperature, Einstein had carried out the following manipulations. Observing that the *Entartung* parameter has to be in principle smaller or equal to one, he had expanded each term of the sum into a power series,

$$n = \sum_S \sum_{\sigma} \lambda^{\tau} \exp\left(-\frac{E_{S\tau}}{kT}\right)$$

and then had replaced the sum over  $s$  by an integration, thus obtaining,

$$n = \frac{(2\pi mkT)^{\frac{3}{2}}}{h^3} V \sum_{\tau} \tau^{-\frac{3}{2}} \lambda^{\tau}$$

He had then noted that this equation expressed an upper limit on the number of particles for a given volume and a given temperature the gas. The maximum number of particle in the gas was given by

$$n_{max} = \frac{(2\pi mkT)^{\frac{3}{2}}}{h^3} V \sum_{\tau} \tau^{-\frac{3}{2}}$$

where the sum in  $\tau$  is just a finite constant. It was at this point that he had asked, “But then what happens if I let the density of the substance increase further at this temperature (for example by isothermal compression)?”, and had asserted that, according to the model of the isothermal compression of a saturated vapour, a separation would take place, and the molecules in excess of the maximum number would “condense” into the quantum state of lowest energy.

### Uhlenbeck’s Criticism

In 1927, Uhlenbeck, then a student of Paul Ehrenfest in Leiden, studied the Fermi-Dirac and the Bose-Einstein statistics, and their relation to the classical Maxwell-Boltzmann statistics for his doctoral thesis. He came to object to Einstein’s prediction of condensation on the following ground. He observed that Einstein’s conclusion was in mathematical contradiction with the fact that the first term of the sum (1), which represented the average number of molecules in the state of zero kinetic energy, became infinite for  $\lambda = 1$ . The appearance of a maximum for the number of gas molecules was caused only by the approximation of the sum by an integral. The exact expression for the number of molecules had no upper limit; on the contrary, it became infinite for  $\lambda \rightarrow 1$ . The value of the *Entartung* parameter was indeed determined by the given number of molecules and temperature, and it was certainly smaller than one for high temperatures and low densities. As the temperature lowered, the lowest quantum states would “be more and more filled, and in much stronger degree than would be the case in Boltzmann statistics.” The *Entartung* parameter could reach the value one only asymptotically, and no “splitting into two phases” would occur.<sup>10</sup>

<sup>9</sup>Einstein, “Quantentheorie” (note 7), on 266. I re-wrote Einstein’s equation in a compact form. See note 7 for Einstein’s original formulae.

<sup>10</sup>G. E. Uhlenbeck, *Over Statistische Methoden in de Theorie der Quanta* (’s Gravenhage: Martinus Nijhoff, 1927), 69–71. I thank Jos Uffink for his help with the original Dutch text.

The criticism came from Leiden, the location of Kamerlingh-Onnes's cryogenic laboratory, powerhouse for the production of new knowledge on condensation phenomena, and the academic home of Paul Ehrenfest. Ehrenfest was the first to whom Einstein had communicated his idea of a "condensation without attractive forces" in a gas governed by Bose's "almost unintelligible" statistics. We know that Ehrenfest was rather sceptical of this new statistical method, which, as Einstein himself admitted, could be justified only *a posteriori* through its success for the radiation law. Possibly, Einstein's had been encouraged in envisioning condensation in such a gas by the fact that, in response to Ehrenfest's criticisms, he had had to recognize that his and Bose's method did not treat the gas molecules as independent. Hence, although there were no attractive forces among molecules, one had to admit a "mutual influence" which was, for the time being, of a "mysterious nature".<sup>11</sup> Ehrenfest was unmoved, and apparently the condensation by mysterious influence did nothing to mitigate his reserves. Not only did Ehrenfest support Uhlenbeck's criticism, but he positively cheered for it, for he wrote his friend Einstein a playful letter in the form of a physics journal article, which began, "Title: Does the Bose-Einstein Statistics Lead for Ideal Gases to a Condensation in the Degenerate State? Summary: No!" In 1933, Ehrenfest published the first attempt at a comprehensive classification of phase transitions. This was his last work before his death. Bose-Einstein condensation was not mentioned in it. But the wind had begun to turn, and Ehrenfest's classification would unintentionally play a major role in reversing the fortune of Einstein's prediction.

### The Reappraisal

In the first place, the advancement of quantum mechanics had dispelled the mystery around the Bose-Einstein gas. In 1926, Paul Dirac had showed that the new quantum statistics, the Bose-Einstein statistics and the one that became known as the Fermi-Dirac statistics, were related to the symmetry of the wave function, and hence to the invariance of observable quantities, under exchanges of particles. This property, which became known as the quantum *indistinguishability* of particles, was adopted as the justification of the appearance of mutual influence among particles subjected to the Bose-Einstein statistics.

Another pivotal development had taken place right in Leiden. It was the immediate motivation of Ehrenfest's re-thinking of phase transitions. Willem Hendrik Keesom, Kamerlingh-Onnes's successor, and his collaborator Mieczyslaw Wolfke observed an abrupt variation in dielectric constant of liquid helium. Added to earlier data about other sharp changes in thermodynamic parameters, the change in dielectric constant suggested a phase transition near the critical temperature  $T_c = 2.2$  K. Keesom and Wolfke hypothesized two phases in liquid helium and called them He-I and He-II. The helium transition was similar to ordinary phase transitions in the sudden jumps that several thermodynamic parameters underwent around the critical temperature, but it differed in that it involved no latent heat and no change in the appearance of the substance. In 1932-33, Keesom and collaborators measured the variation of specific heat with temperature around the critical temperature, and published a curve which showed a characteristic, very marked jump. Keesom took up a suggestion from Ehrenfest and

---

<sup>11</sup>Einstein, "Quantentheorie. Zweite Abhandlung" (note 6), on 6.

called the critical temperature “the lambda point” because of the shape of the curve. The transition became known as “the lambda transition”.

The existing theoretical treatment of phase transitions was a combination of the van der Waals equation and Gibbs’s conditions of thermodynamic equilibrium of coexisting phases. A process like the lambda transition was not contemplated in it. Ehrenfest formulated a characterization of phase transitions capable of including ordinary phase transitions and the lambda transition, as well as other critical phenomena such as the magnetization of ferromagnetic materials and superconductivity. He defined a phase transition as an analytic discontinuity in the derivatives of the Gibbs free energy,  $G = U - TS + pV$ . He then classified processes as being of the first order if they corresponded to a discontinuity of the first derivative, of the second order if they corresponded to a discontinuity of the second derivative, and so on. Accordingly, ordinary changes of state such as gas to liquid were first order transitions because in them the entropy and the volume, first derivatives of the Gibbs free energy, were discontinuous. In the lambda transition, entropy and volume did not change, but the specific heat, a second derivative of the Gibbs free energy, had a jump, so the lambda transition was a second order transition. The scheme made room naturally for hypothetical transitions of higher orders.

The Ehrenfest classification was a very influential attempt at ordering the growing variety of critical processes under a general definition based on the mathematical properties of thermodynamic functions. It has been described as a major step toward the creation of a new area of study concerned with “cooperative phenomena”.<sup>12</sup> These are a subclass of the phenomena pertaining to large assemblies of particles. They are defined as those phenomena in which the states of the assembly are not related in a simple manner to the states of the individual particles because the particles are strongly correlated. Understood as cooperative phenomena in this sense, phase transitions are regarded as paradigmatic of the emergent properties of complex systems.<sup>13</sup> But a subfield centred on this negative definition could only form by differentiating itself from a field founded upon the assumption that large assemblies of particles do have states that can be understood in terms of the states of the individual components. To be more specific, a theoretical understanding of phase transitions as cooperative phenomena required a general statistical mechanical derivation of thermodynamics as a precondition.<sup>14</sup>

Uhlenbeck’s reconsideration of his objection to Bose-Einstein condensation was inspired by the first statistical-mechanical theory of condensation, which was formulated in 1937 by the American physical chemist Joseph E. Mayer. Mayer had begun his career at the school of physical chemistry headed by Gilbert N. Lewis in Berkeley. Physical chemistry in those days was, according to Mayer, “almost exclusively the application of

---

<sup>12</sup>L. Hoddeson et al., “Collective Phenomena”, in L. Hoddeson et al., eds., *Out of the Crystal Maze. Chapters from the History of Solid-State Physics* (New York: Oxford University Press, 1992), 489–598. Hoddeson et al. attribute the explicit definition of the statistical mechanical study of cooperative phenomena as a separate subfield to R. H. Fowler, in the 1936 edition of his *Statistical Mechanics*.

<sup>13</sup>See, for example, Philip W. Anderson, “More is Different”, *Science* 177, 4047 (1972), 393–396.

<sup>14</sup>My observation is limited to the statistical definition of cooperative phenomena, which consists of the denial of an otherwise underlying assumption in statistical mechanics. For an history and analysis of early notions of “collectivized entities”, that is, individual electrons that are neither “free” nor “bound” to single atoms in solids, or quantized collective excitations, see A. Kojevnikov, “Freedom, collectivism, and quasiparticles: Social metaphors in quantum physics”, *Historical Studies in the Physical and Biological Sciences*, 29 (1999), 295–331.

thermodynamics.” Mayer and Lewis undertook a systematic study of statistical mechanics in 1928. Here is Mayer’s account of his encounter with this discipline:

I had no knowledge of statistical mechanics and Lewis had never worked in the field either. He had become interested in the discovery that had just been made of the difference between quantum mechanical statistical mechanics and the classical, and the Bose-Einstein versus the Fermi-Dirac systems. During the day I tried to learn statistical mechanics... Gilbert and I spent the evening together... I still like the methods that we evolved for deriving thermodynamics from statistical mechanics, that is, from the mechanical laws for the motion of molecules.<sup>15</sup>

The result of this effort was a series of papers on the derivation of thermodynamics from statistical mechanics by Lewis and Mayer (Lewis and Mayer, 1928, 1929). The last of the Lewis and Mayer papers dealt with quantum statistics; notably, however, it makes no mention of Bose-Einstein condensation.

In 1937, Mayer wrote, in collaboration with two of his students, “an epochmaking series of papers” which were titled “The Statistical Mechanics of Condensing Systems”.<sup>16</sup> In these, he developed a method for deriving the thermodynamic quantities of systems of interacting particles, that is, real systems, starting from simple assumptions about the inter-particle potential. The method used a series expansion of the partition function, in which the first term corresponded to the non-interacting (ideal) gas, and the subsequent terms represented the corrections arising from the interactions. Mayer’s method is known as the “method of cluster expansions” because it decomposes the effects of particle-particle interactions in terms of a two-particle function and its two-fold, three-fold, etc. products, each of which can be interpreted as representing a cluster of two, three, etc. particles. The cluster terms will depend on the volume  $V$  of the system in a way that can be interpreted as a “surface effect”. In the limit of infinite volume, they have a finite value that depends on the temperature. Therefore, the equation of state of the interacting system can be written, in the limit  $V \rightarrow \infty$ , as

$$\frac{P\nu}{kT} = \sum_{l=1}^{\infty} a_l(T) \left( \frac{\lambda_{dB}^3}{\nu} \right)^{l-1}$$

where  $\nu = \frac{V}{n}$  is the volume per particle in the system, and  $\lambda_{dB}$  is the parameter called *mean thermal wavelength*, or *thermal de Broglie wavelength* of the particles in the system, and is defined as  $\lambda_{dB} \equiv \left( \frac{h}{2\pi m k T} \right)^{\frac{1}{2}}$ . This form of the state equation is known as the *virial expansion* of the system, and the  $a_l(T)$  are called *virial coefficients*.

Max Born regarded Mayer’s theory of condensation “as a most important contribution to statistical mechanics,” and presented it at an international conference that was

<sup>15</sup>Joseph E. Mayer, “The Way It Was”, *Annual Review of Physical Chemistry*, 33 (1982), 1–23, on 9 and 13–14.

<sup>16</sup>Bruno H. Zimm, “Joseph Edward Mayer”, *Biographical Memoirs of the National Academy of Sciences*, 65 (1994), 211–220, on 213. J. E. Mayer, “The Statistical Mechanics of Condensing Systems. I”, *Journal of Chemical Physics*, 5 (1937), 67–73; J. E. Mayer and P. G. Ackermann, “The Statistical Mechanics of Condensing Systems. II”, *Journal of Chemical Physics*, 5 (1937), 74–83; J. E. Mayer and S. F. Harrison, “The Statistical Mechanics of Condensing Systems. III”, *Journal of Chemical Physics*, 6 (1938), 87–100; S. F. Harrison and J. E. Mayer, “The Statistical Mechanics of Condensing Systems. IV”, *Journal of Chemical Physics*, 6 (1938), 101–104.

held in Amsterdam in late 1937 for the van der Waals's centenary.<sup>17</sup> Since, however, he found Mayer's treatment obscure and somewhat unconvincing, he undertook a systematization and clarification of it in collaboration with Klaus Fuchs. Meanwhile, he was corresponding with Uhlenbeck, who had also become interested in Mayer's work.

Mayer's theory and Born's elaboration of it dealt with a classical system. Uhlenbeck and his student Boris Kahn extended it to quantum statistics. Furthermore, they were able to modify the method so that it could be also applied to an ideal gas. In particular, Kahn and Uhlenbeck noticed a strong formal analogy between the virial expansion of Mayer's theory and Einstein's series expansions, and between Mayer's and Einstein's arguments for condensation. A physical interpretation of the analogy was enabled by a result obtained by Uhlenbeck in 1932, according to which the assumption of Bose-Einstein statistics was equivalent to the assumption of "quasiattractive forces" among the molecules.<sup>18</sup> Having simplified Mayer's forbidding formalism, Uhlenbeck and Kahn obtained formulae for the density and pressure of the non-ideal gas that were "identical with Einstein's equations" for the ideal gas. They wrote,

Einstein has already shown that these equations describe a condensation phenomenon. In fact the series for  $N$  converges for the maximum value of  $A$  and there exist therefore a maximum density. For smaller volumes a certain number of molecules will condense into the state of zero energy, and the pressure remains constant.<sup>19</sup>

Uhlenbeck and Kahn repeated Uhlenbeck's earlier remark, that Einstein's formulae were valid only if one neglected the quantization of the translational energy of the molecules. They endorsed Mayer's argument for condensation adducing that it coincided with the argument given by Einstein for the ideal gas, even though they still considered Einstein's formulae inapplicable. In turn, as we will see, Mayer's theory and the reflections that it stirred would afford Uhlenbeck and Kahn the means to rehabilitate Einstein's formulae. The argument, as they articulated it, consisted of two points. The first was that for a given volume the number of particles of the gas had a finite maximum. The reaching of the maximum would mark the saturation point, beyond which the molecules in excess would begin to accumulate in the state of zero energy. The second was that the pressure of the gas would remain constant as the volume decreased beyond the saturation point, as was expected in a condensation process. Even though Kahn and Uhlenbeck attributed the reasoning to Einstein and Mayer, only the first of the two points had been presented by Einstein in the 1925 paper. And only the second had been part of Mayer's discussion of how to read the occurrence of condensation out of his involved mathematical formalism.

Born, and Kahn and Uhlenbeck's treatments of condensing systems caused a "vigorous discussion" at the Amsterdam conference, "on the question as to whether Mayer's

---

<sup>17</sup>Max Born and Klaus Fuchs, "The Statistical Mechanics of Condensing Systems", *Proceedings of the Royal Society of London*, A166 (1938), 391–414, on 391; Max Born, "The Statistical Mechanics of Condensing Systems", *Physica*, 4 (1937), 1034–1044.

<sup>18</sup>B. Kahn and G. E. Uhlenbeck, "On the theory of condensation", *Physica*, 4 (1937), 1155–1156, on 1155; G. E. Uhlenbeck and L. Gropper, "The Equation of State of a Non-ideal Einstein-Bose or Fermi-Dirac Gas", *Physical Review*, 41 (1932), 79–90.

<sup>19</sup>B. Kahn and G. E. Uhlenbeck, "On the theory of condensation", *Physica*, 4 (1937), 1155–1156, on 1155. Kahn and Uhlenbeck's parameter  $A$  is  $A = \frac{\lambda}{\lambda_{dB}^3}$

explanation of the phenomena of condensation is correct.”<sup>20</sup> By this time, following the Ehrenfest classification, phase transitions had come to be defined as analytical discontinuities in thermodynamic functions. At the same time, it had become self-evident that the thermodynamic functions of a system were to be derived from its statistical mechanics. A conflict arose, for it was difficult to see how one could obtain analytical discontinuities from the partition function of a system of particles, which was thoroughly analytic. The debate was so undecided that the question was put to vote, and the votes turned out to be evenly divided. Here is how Uhlenbeck later recounted this episode:

Can one prove with mathematical rigor from the foundations of statistical mechanics, i.e. from the partition function, that a gas with given intermolecular forces will condense at sufficiently low temperature at a sharply defined density, so that the isotherms will exhibit a discontinuity? It may seem strange now that there could be any doubt that this would be possible but at the Conference (so still in 1937!) one wasn't so sure and I remember that Debye, for instance, doubted it. In my opinion, the liberating word was spoken by Kramers. He remarked that a phase transition (such as condensation) could mathematically only be understood as a limiting property of the partition function. Only in the limit, where the number of molecules  $N$  and the volume  $V$  go to infinity such that  $N/V$  remains finite (one calls this now the thermodynamic limit) can one expect that the isotherm will exhibit the two known discontinuities.<sup>21</sup>

Kahn and Uhlenbeck embraced Kramers's proposal, which allowed them to reconcile Ehrenfest's definition of phase transitions with their belief that the statisticalmechanical partition function contained “all possible states of a system”. They converted to the idea that a mathematical description of phase transitions could only be obtained in the limit of infinite volume and infinite number of particles, with the density remaining finite, and that the physical sense of such operation would be recovered by stating that “the problem has only physical sense when  $N$  is very large.”<sup>22</sup> This new logic entailed a tacit reversal of position. Ten years earlier Uhlenbeck had maintained that, since the *Entartung* parameter of Einstein's gas would approach the value one without ever reaching it, a splitting of the gas into two phases would not occur. Now, he and Kahn were ready to champion the new understanding of phase transitions as “limit properties”, and hence to accept that also in an ideal Bose-Einstein gas condensation would occur in the thermodynamic limit.

Deepening the analogy between Mayer's and Einstein's theories, Kahn and Uhlenbeck were able to adapt the cluster summation to the ideal gas and to derive the condensation formulae with a “strict calculation” that avoided the questionable approximation used by Einstein. They stressed, however, that Einstein's and Mayer's arguments for condensation were incomplete.

Comparing the thermodynamic functions obtained in Mayer's and Einstein's case with those of the Fermi-Dirac statistics, Uhlenbeck and Kahn came to the conclusion that condensation would occur in Mayer's and in Einstein's gases, but not in a Fermi-Dirac

---

<sup>20</sup>Born and Fuchs, “The statistical mechanics of condensing systems” (note 17), on 391.

<sup>21</sup>Uhlenbeck, quoted in Cohen, “George E. Uhlenbeck and statistical mechanics” (note 3), on 619.

<sup>22</sup>B. Kahn and G. E. Uhlenbeck, “On the Theory of Condensation”, *Physica*, 5 (1938), 399–415, on 401.



gas. Along with the recursive application of the formal analogy between the Bose-Einstein ideal gas and Mayer's real gas, the crucial ingredient of this conclusion was an enlarged notion of condensation according to Ehrenfest's definition of phase transitions, complemented by the idea of phase transitions as "limit properties". Uhlenbeck and Khan pointed out that Einstein's condensation would have "some uncommon features"; for instance, the isothermal variation of the pressure with the volume would have no discontinuity at the critical point.<sup>23</sup> Nonetheless, in the Mayer and Einstein cases the value one of the Entartung parameter would represent a singular point for density and pressure, while it would not represent a singular point in the Fermi-Dirac case. In the same vein, shortly later Fritz London would observe that the condensation of the Bose-Einstein gas represented "a discontinuity of the derivative of the specific heat (phase transition of the third order)."<sup>24</sup>

## Conclusion

To summarize, the first theory of phase transitions founded on classical statistical mechanics was produced by a physical chemist, who had trained himself in statistical mechanics in the wake of enthusiasm and curiosity that followed the birth of quantum statistics and quantum mechanics. This theory, in turn, led to a systematic re-formulation, on the basis of a quantum statistical method and a new definition of phase transitions, of Einstein's argument for condensation in an ideal gas. From this outline of the story of the early days of Bose-Einstein condensation, it would seem that, contrary to the suggestions implied by the terminology of "classical" statistics and quantum "revolution", quantum statistical mechanics did not come to overthrow and supplant a normal-science regime of classical statistical mechanics. It arrived, rather, at a stage in which statistical mechanics was itself young, and the classical and quantum branches of it developed to a considerable extent in parallel, or better, interacting with each other.

In the way of conclusion I shall formulate two questions for my ongoing research. How much did the advent of quantum mechanics and quantum statistics influence, or even favour, the widespread adoption of statistical mechanics as the effective foundation of thermodynamics? And how much did Bose-Einstein condensation, being the first phase transition fully rooted in the statistical treatment of a thermodynamic system, contribute to the emergence of the new category of "cooperative phenomena"?

---

<sup>23</sup>Kahn and Uhlenbeck, "On the Theory of Condensation" (note 22), on 408–409.

<sup>24</sup>F. London, "The  $\lambda$ -Phenomenon in Liquid Helium and the Bose-Einstein Degeneracy", *Nature*, 141 (1938), 643–644, on 644.

# 10 Pascual Jordan's Resolution of the Conundrum of the Wave-Particle Duality of Light

ANTHONY DUNCAN AND MICHEL JANSSEN

*In 1909, Einstein derived a formula for the mean square energy fluctuation in black-body radiation. This formula is the sum of a wave term and a particle term. In a key contribution to the 1926 Dreimännerarbeit with Born and Heisenberg, Jordan showed that one recovers both terms in a simple model of quantized waves. So the two terms do not require separate mechanisms but arise from a unified dynamical framework. In this paper, we give a detailed reconstruction of Jordan's derivation of this result and discuss the curious story of its reception. Several authors have argued that various infinities invalidate Jordan's result. We defend it against such criticism. In particular, we note that the fluctuation in a narrow frequency range, which is what Jordan calculated, is perfectly finite. We also note, however, that Jordan's argument is incomplete. In modern terms, Jordan calculated the quantum uncertainty in the energy of a subsystem in an energy eigenstate of the whole system, whereas the thermal fluctuation is the average of this quantity over an ensemble of such states. Still, our overall conclusion is that Jordan's argument is basically sound and that he deserves more credit than he received for having resolved a major conundrum in the development of quantum physics.*

## 10.1 The Recovery of Einstein's Fluctuation Formula in the Dreimännerarbeit

In the final section of the famous *Dreimännerarbeit* of Max Born, Werner Heisenberg, and Pascual Jordan (1926), the *Umdeutung* [= reinterpretation] procedure of (Heisenberg, 1925) is applied to a simple system with infinitely many degrees of freedom, a continuous string fixed at both ends. In a lecture in Göttingen in the summer of 1925 (p. 380, note 2)<sup>1</sup>—attended, it seems, by all three authors of the *Dreimännerarbeit*—Paul Ehrenfest (1925) had used this system as a one-dimensional model for a box filled with black-body radiation and had calculated the mean square energy fluctuation in a small segment of it. The string can be replaced by an infinite set of uncoupled harmonic oscillators, one for each mode of the string. The harmonic oscillator is the simplest application of Heisenberg's new quantum-theoretical scheme. The basic idea behind this scheme was to retain the classical equations of motion but to *reinterpret* these equations—hence the term *Umdeutung*—as expressing relations between arrays of numbers, soon to be recognized as matrices (Born and Jordan, 1925), assigned not to individual states but to

<sup>1</sup>Unless noted otherwise, references are to (Born, Heisenberg, and Jordan, 1926).

transitions between them and subject to a non-commutative multiplication law.<sup>2</sup> When this *Umdeutung* procedure is applied to the harmonic oscillators representing the modes of a string and the mean square energy fluctuation in a small segment of the string and in a narrow frequency interval is calculated, one arrives at a surprising result. In addition to the classical wave term, proportional to the square of the mean energy, one finds a term proportional to the mean energy itself. This term is just what one would expect for a system of particles.

For this simple model, one thus recovers both terms of Albert Einstein's well-known formula for the mean square energy fluctuation in a narrow frequency range in a small subvolume of a box with black-body radiation. As Einstein showed in 1909, this formula is required by Planck's law for the spectral distribution of black-body radiation and some general results in statistical mechanics. As Martin J. Klein (1970) characterized the situation: "Einstein concluded that there were two independent causes producing the fluctuations, and that an adequate theory of radiation would have to provide both wave and particle mechanisms" (p. 6). The derivation in the *Dreimännerarbeit* shows, contrary to Einstein's expectation, that both terms in the fluctuation formula can be accounted for within a unified dynamical framework.

The authors presented their unified mechanism in terms of (quantized) waves, but it can also be described in terms of (quantum) particles. Heisenberg (1930) stated this explicitly a few years later: "The quantum theory, which one can interpret as a particle theory or a wave theory as one sees fit, leads to the complete fluctuation formula" (p. 101; see also, e.g., Jordan, 1936, p. 220). The result thus illustrates the kind of wave-particle duality associated with Niels Bohr's notion of complementarity, which is different from the kind originally envisioned by Einstein. It does not involve the coexistence of two different mechanisms but the existence of one that can be described in different ways. While illustrating one aspect of complementarity, the fluctuation formula undermines another. A quantum system is supposed to present itself to us either under the guise of waves or under the guise of particles, depending on the experimental context. However, if one were to measure the mean square energy fluctuation in a small subvolume of a box with black-body radiation, as one probably could even though Einstein conceived of it only as a thought experiment, and Einstein's formula is correct, which is no longer in any serious doubt,<sup>3</sup> one would see the effects of waves and particles simultaneously.<sup>4</sup>

One might have expected that the recovery of Einstein's fluctuation formula in the *Dreimännerarbeit* would have been hailed right away as the triumphant resolution of a major conundrum in the development of quantum physics; and that it would since have become a staple of historical accounts of the wave-particle duality of light. Both expectations prove to be wrong. As we shall see in sec. 10.3, Jordan was responsible for this part of the *Dreimännerarbeit* and even his co-authors were skeptical about the result.<sup>5</sup> To give an example from the historical literature, Klein's (1964) classic paper,

---

<sup>2</sup>See (Duncan and Janssen, 2007) both for an account of what led Heisenberg to this idea and for further references to the extensive historical literature on this subject.

<sup>3</sup>*Pace* (Gonzalez and Wergeland, 1973).

<sup>4</sup>We owe this last observation to Jos Uffink (private communication). For discussion of the differences between Heisenberg's wave-particle equivalence and Bohr's wave-particle complementarity, see (Camilleri, 2006).

<sup>5</sup>More recently, physicists have recognized the importance of Jordan's result (see, e.g., Weinberg, 1977, 1995; Wightman, 1996; Cini, 2003).

“Einstein and the wave-particle duality,” does not even cite the *Dreimännerarbeit*.<sup>6</sup> To the best of our knowledge, the only Einstein biography that touches on the derivation of the fluctuation formula in the *Dreimännerarbeit* is the one by Abraham Pais (1982, p. 405). The canonical twin stories of the light-quantum hypothesis and the wave-particle duality of light end with the Compton effect and Bohr complementarity, respectively. The canonical history fails to mention that the specific challenge posed by Einstein's fluctuation formula, which suggested wave-particle duality in the first place, was taken up and, we want to argue, convincingly met in the *Dreimännerarbeit*.<sup>7</sup> It also tends to ignore the difference noted above between Einstein's original conception of wave-particle duality and wave-particle duality as it is usually understood in quantum mechanics (see, e.g., Pais, 1982, p. 404).

Having chastised historians of physics in such broad-brush fashion, we hasten to add that ours is certainly not the first contribution to the historical literature that draws attention to the fluctuation calculations in the *Dreimännerarbeit*. For instance, even though Klein (1980) did not mention these calculations in his lecture at the Princeton Einstein centenary symposium, John Stachel, director of the Einstein Papers Project at the time, did bring them up in question time (Woolf, 1980, p. 196). Stachel also drew attention to correspondence between Einstein and Jordan pertaining to these calculations. Unfortunately, most of Einstein's letters to Jordan have not survived.<sup>8</sup> Jagdish Mehra and Helmut Rechenberg (1982–2001, Vol. 3, pp. 149–156) devote a section of their comprehensive history of quantum mechanics to this part of the *Dreimännerarbeit*, although they offer little assistance to a reader having difficulties following the derivation. The relevant section of the *Dreimännerarbeit* also plays a central role in a paper on Einstein's fluctuation formula and wave-particle duality by Alexei Kojevnikov (1990); in a recent paper on Jordan's contributions to quantum mechanics by Jürgen Ehlers (2007); and in a paper on the origin of quantized matter waves by Olivier Darrigol (1986). This last author clearly shares our enthusiasm for these fluctuation calculations, calling them “spectacular” at one point and stressing that they formed the solution to “the most famous puzzle of radiation theory” (ibid., p. 221–222).

---

<sup>6</sup>The same is true for Klein's (1979, 1980, 1982) contributions to three volumes published in connection with the centenary of Einstein's birth, even though the first briefly touches on Einstein's reaction to matrix mechanics (Klein, 1979, p. 149) and the third is specifically on Einstein and fluctuations. In a much earlier paper on Ehrenfest, Klein (1959, p. 50) mentioned the importance of (Ehrenfest, 1925) for this part of the *Dreimännerarbeit*, but added, contrary to what we shall argue, that “a satisfactory discussion of the “mechanism” of the fluctuations” was not given until (Heisenberg, 1931).

<sup>7</sup>Another episode in the history of Einstein and wave-particle duality that seldom gets attention is the one involving the fraudulent canal ray experiments of Emil Rupp (Van Dongen, 2007a,b).

<sup>8</sup>In response to a query by Stachel, Jordan wrote, whitewashing his own involvement with the Nazis in the process: “Indeed those letters the loss of which I mention in [Jordan, 1969, p. 55] are really destroyed and there is no hope that they could be still discovered anywhere. Perhaps you may be astonished that I did not strive more earnestly to preserve them. But you must understand that only the fact of keeping in my house a series of kind and personal letters of Einstein meant a condition of permanent danger under the circumstances in which I had to live here for “1000 years”. Being criticized by Lenard and other political enemies of modern physics as a dangerous follower of Einstein and other antagonists of the Hitler Empire I was forced to await every day the possibility that a police-examination of my papers could be performed and finding there the letters from Einstein might result in my immediate arrest. During the war this danger became still more threatening. Therefore the letters must not only been kept, but they must remain hidden in an appropriate manner, and that was bad for preserving them in cases of air-attack in the night” (Jordan to Stachel, April 14, 1978, typed in imperfect English [Einstein Archive (AE), 75–274]).

Aside from a preamble on Einstein’s fluctuation formula and its early history (sec. 10.2) and a brief conclusion (sec. 10.5), our paper is divided into two longer sections, one historical and one technical (secs. 10.3–4). In the latter, we give a detailed and self-contained reconstruction of the calculation in the *Dreimännerarbeit* of the mean square energy fluctuation in a small segment of a string, Ehrenfest’s simple one-dimensional model for a subvolume of a box filled with black-body radiation. This fills an important gap in the historical literature. Our reconstruction will enable us to defend the derivation against various criticisms and it will enable readers to assess such criticisms and our rejoinders for themselves. In the historical section (sec. 10.3), which draws both on the work of Darrigol and Kojevnikov and on the results of our own reconstruction of the calculations, we explore the question why the recovery of Einstein’s fluctuation formula in the *Dreimännerarbeit* is not nearly as celebrated as one might have expected it to be.

## 10.2 Einstein, Fluctuations, and Wave-Particle Duality

In a fifty-page semi-popular history of the light-quantum hypothesis, Jordan (1928, pp. 162–163)<sup>9</sup> distinguished between “Einstein’s first fluctuation formula” and “Einstein’s second fluctuation formula.”<sup>10</sup> The former is derived in the paper introducing light quanta. Einstein (1905) considered black-body radiation in the Wien regime of high frequencies in a box of volume  $V_0$ . He imagined a fluctuation as a result of which, for a brief moment, all energy  $E$  of the radiation in a narrow frequency range around  $\nu$  gets concentrated in a subvolume  $V$ . Using Boltzmann’s relation between entropy and probability, Einstein showed that the probability of this fluctuation is given by  $(V/V_0)^{E/h\nu}$  (where, unlike Einstein in 1905, we used Planck’s constant  $h$ ). For an ideal gas of  $N$  particles in a box of volume  $V_0$ , the probability of a fluctuation such that all particles momentarily end up in a subvolume  $V$  is given by  $(V/V_0)^N$ . Comparing the two expressions, Einstein (1905) concluded that “monochromatic radiation [in the Wien regime] behaves thermodynamically as if it consisted of  $[N]$  mutually independent energy quanta of magnitude  $[h\nu]$ ” (p. 143).

The *Dreimännerarbeit* is concerned with Einstein’s second fluctuation formula. This formula does not give the probability of a specific fluctuation but the mean square energy fluctuation of black-body radiation in a narrow frequency range in some subvolume. Statistical mechanics gives the following general formula for the mean square energy fluctuation:

$$\langle \Delta E^2 \rangle = kT^2 \frac{d\langle E \rangle}{dT}, \quad (10.1)$$

where  $k$  is Boltzmann’s constant,  $T$  is the temperature, and  $\langle E \rangle$  is the mean energy. Einstein (1904) derived this formula in the concluding installment of his so-called “statistical trilogy.” Unbeknownst to him, it had already been published in 1902 by Josiah W. Gibbs. Einstein (1904, sec. 5), however, was the first to apply it to black-body radiation. A few years later, Einstein (1909a,b) returned to these considerations. As

<sup>9</sup>Jordan sent an offprint of this article to Einstein (Jordan to Einstein, November 23, 1928 [AE 13–476]). From a letter three weeks later (Jordan to Einstein, December 11, 1928 [AE 13–477]), it can be inferred that Einstein replied with a long letter. This letter has not survived (see note 8) and Jordan’s response is of little help in reconstructing its contents.

<sup>10</sup>See (Norton, 2006; Rynasiewicz and Renn, 2006; Uffink, 2006) for recent discussions of Einstein’s early use of fluctuation arguments.

Klein (1964) writes: “instead of trying to derive the distribution law from some more fundamental starting point [as Max Planck had done in 1900], ... [Einstein] assume[d] its correctness and [saw] what conclusions it implied as to the structure of radiation” (p. 9). In the special case of black-body radiation, there is a “frequency specific version” (Rynasiewicz and Renn, 2006, p. 19) of Eq. (10.1):

$$\langle \Delta E_\nu^2 \rangle = kT^2 \frac{d\langle E_\nu \rangle}{dT} = kT^2 \frac{\partial \rho(\nu, T)}{\partial T} V d\nu, \quad (10.2)$$

where  $\langle E_\nu \rangle = \rho(\nu, T) V d\nu$  is the mean energy of the black-body radiation in the frequency range  $(\nu, \nu + d\nu)$  at temperature  $T$  in the subvolume  $V$ .  $\langle \Delta E^2 \rangle$  is the integral of  $\langle \Delta E_\nu^2 \rangle$  over all frequencies. By inserting the Rayleigh-Jeans law, the Wien law, and the Planck law (denoted by the subscripts ‘RJ’, ‘W’, and ‘P’) for  $\rho(\nu, T)$  in Eq. (10.2), we find the formula for  $\langle \Delta E_\nu^2 \rangle$  predicted by these three laws ( $c$  is the velocity of light):

$$\begin{aligned} \rho_{\text{RJ}} &= \frac{8\pi}{c^3} \nu^2 kT, & \langle \Delta E_\nu^2 \rangle_{\text{RJ}} &= \frac{c^3}{8\pi\nu^2} \frac{\langle E_\nu \rangle_{\text{RJ}}^2}{V \Delta\nu}; \\ \rho_{\text{W}} &= \frac{8\pi h}{c^3} \nu^3 e^{-h\nu/kT}, & \langle \Delta E_\nu^2 \rangle_{\text{W}} &= h\nu \langle E_\nu \rangle_{\text{W}}; \\ \rho_{\text{P}} &= \frac{8\pi h}{c^3} \frac{\nu^3}{e^{h\nu/kT} - 1}, & \langle \Delta E_\nu^2 \rangle_{\text{P}} &= \frac{c^3}{8\pi\nu^2} \frac{\langle E_\nu \rangle_{\text{P}}^2}{V \Delta\nu} + h\nu \langle E_\nu \rangle_{\text{P}}. \end{aligned} \quad (10.3)$$

For the Rayleigh-Jeans law,  $\langle \Delta E_\nu^2 \rangle$  is proportional to the square of the mean energy. To borrow a phrase from John Norton (2006, p. 71), this is the *signature of waves*. For the Wien law,  $\langle \Delta E_\nu^2 \rangle$  is proportional to the mean energy itself. This is the *signature of particles*. For the Planck law—originally obtained through interpolation between the Wien law and (what became known as) the Rayleigh-Jeans law— $\langle \Delta E_\nu^2 \rangle$  has both a wave and a particle term.

In a lecture at the 1909 Salzburg *Naturforscherversammlung*, Einstein (1909b) famously prophesized on the basis of this last formula and a similar one for momentum fluctuations “that the next phase of the development of theoretical physics will bring us a theory of light that can be interpreted as a kind of fusion of the wave and emission theories” (pp. 482–483). Contrary to what the term “fusion” [*Verschmelzung*] in this quotation suggests, Einstein believed that his fluctuation formulae called for two separate mechanisms: “the effects of the two causes of fluctuation mentioned [waves and particles] act like fluctuations (errors) arising from *mutually independent causes* (additivity of the terms of which the square of the fluctuation is composed)” (Einstein, 1909a, p. 190, our emphasis).<sup>11</sup> This was still Einstein’s view in the early 1920s. As he wrote to Arnold Sommerfeld on October 9, 1921: “I am convinced that some kind of spherical wave is emitted *besides* the directional energetic process” (Einstein, 1987–2006, Vol. 7, p. 486; our emphasis).

Reluctant to abandon the classical theory of electromagnetic radiation and to embrace Einstein’s light-quantum hypothesis, several physicists in the 1910s and early 1920s tried either to poke holes in Einstein’s derivation of the (energy) fluctuation formula so that

---

<sup>11</sup>See also (Einstein 1909b, p. 498; 1914, p. 346), the quotation from (Klein, 1970) in the introduction, and the discussion in (Bach, 1989, p. 178).

they could avoid the formula or to find an alternative derivation of it that avoided light quanta.<sup>12</sup> In the wake of the discovery of the Compton effect and of Satyendra Nath Bose's (1924) new derivation of Planck's black-body radiation law, however, both Einstein's fluctuation formula and his light quanta began to look more and more inescapable. The problem of reconciling the wave and the particle aspects of light thus took on greater urgency. In the paper that provided the simple model of a string used in the *Dreimännerarbeit*, for instance, Ehrenfest (1925) emphasized the paradoxical situation that quantizing the modes of a classical wave according to a method proposed by Peter Debye (1910) gives the correct Planck formula for the spectral distribution of black-body radiation but the wrong formula for the mean square energy fluctuation (Stachel, 1986, p. 379). This problem is also highlighted in the *Dreimännerarbeit* (p. 376). As Einstein characterized the situation in an article on the Compton effect in the *Berliner Tageblatt* of April 20, 1924: "There are . . . now two theories of light, both indispensable and—as one must admit today despite twenty years of tremendous effort on the part of theoretical physicists—without any logical connection."<sup>13</sup>

One possibility that was seriously considered at the time, especially after the decisive refutation in April 1925 of the theory of Bohr, Kramers, and Slater (1924a), was that light consisted of particles guided by waves (Duncan and Janssen, 2007, sec. 4.2). In this picture, the waves and the particles presumably give separate contributions to the mean square energy fluctuation, just as Einstein had envisioned. A derivation of Einstein's fluctuation formula based on this picture (and Bose statistics) was given by Walther Bothe (1927).<sup>14</sup> At that point, however, the *Dreimännerarbeit*, which is not cited in Bothe's paper, had already shown that the two terms in the fluctuation formula do not require separate mechanisms after all, but can be accounted for within a single unified dynamical framework.<sup>15</sup>

### 10.3 Why Is the Solution to Einstein's Riddle of the Wave-Particle Duality of Light in the *Dreimännerarbeit* Not Nearly as Famous as the Riddle Itself?

#### 10.3.1 One of Jordan's Most Important Contributions to Physics

The derivation of the fluctuation formula in the *Dreimännerarbeit*, though presented as part of a collaborative effort, was actually the work of just one of the authors, namely Jordan, "the unsung hero among the creators of quantum mechanics" (Schweber, 1994, p. 5). Today, Jordan is mostly remembered as perhaps the only first-tier theoretical

---

<sup>12</sup> For historical discussion and further references, see (Bach, 1989) and (Kojevnikov, 1990). For some brief comments, see (Jordan, 1927b, p. 642, note 2), (Born and Jordan, 1930, p. 398, note 1), and (Jordan, 1936, p. 220).

<sup>13</sup> This often-quoted passage can be found, for instance, in (Pais, 1980, 211; 1982, p. 414; 1986, p. 248), (Klein, 1980, p. 182), and (Bach, 1989, p. 182).

<sup>14</sup> Two earlier papers by Bothe (1923, 1924) and a related paper by Mieczyslaw Wolfke (1921) are cited in the *Dreimännerarbeit* (p. 379, notes 2 and 3).

<sup>15</sup> Independently of full-fledged quantum mechanics and using only Bose's quantum statistics, Reinhold Fürth (1928, p. 312) argued that the fluctuation formula was compatible with waves, particles, or a combination of both. After fleeing Czechoslovakia in 1938, Fürth worked with Born in Edinburgh. In his memoirs, Born (1978, p. 289) praised Fürth's work on fluctuations.

physicist who sympathized strongly and openly with the Nazi ideology.<sup>16</sup> It is hard to say whether this entanglement has been a factor in the neglect of the derivation of the fluctuation formula in the *Dreimännerarbeit*. Our impression is that it only played a minor role. For one thing, it was not until 1930 that Jordan began to voice his Nazi sympathies in print and then only under the pseudonym of Ernst Domaier (Beyler, 2007, p. 71). A much more important factor, it seems, was that Jordan's result immediately met with resistance, even from his co-authors. Right from the start a cloud of suspicion surrounded the result and that cloud never seems to have lifted.<sup>17</sup> Our paper can be seen as an attempt to disperse it.

Except for a short period of wavering in 1926, Jordan steadfastly stood by his result and considered it one of his most important contributions to quantum mechanics. He said so on a number of occasions. One such occasion was a conference in honor of Paul A. M. Dirac's 70th birthday. At the conference, Jordan talked about "the expanding earth" (Mehra, 1973, p. 822), a topic that apparently occupied him for 20 years (Kundt, 2007, p. 124). For the proceedings volume, however, he submitted some reminiscences about the early years of quantum mechanics. There he wrote:

Another piece in the 'Dreimänner Arbeit' gave a result, which I myself have been quite proud of: It was possible to show that the laws of fluctuations in a field of waves, from which Einstein derived the justification of the concept of corpuscular light quanta, can be understood also as consequences of an application of quantum mechanics to the wave field (Jordan, 1973, p. 296).

In the early 1960s, Jordan had likewise told Bartel L. van der Waerden that he "was very proud of this result at the time," adding that he "did not meet with much approval."<sup>18</sup> In a follow-up letter, Jordan wrote:

What [Born and Jordan 1925] says about radiation is not very profound. But what the *Dreimännerarbeit* says about energy fluctuations in a field of quantized waves is, in my opinion, *almost the most important contribution I ever made to quantum mechanics*.<sup>19</sup>

Jürgen Ehlers (2007), who studied with Jordan, relates: "In the years that I knew him, Jordan rarely talked about his early work. On a few occasions, however, he did tell me that he was especially proud of having derived Einstein's fluctuation formula . . . by quantizing a field" (p. 28).

In late 1925, when the *Dreimännerarbeit* was taking shape, Jordan was probably the only physicist who had done serious work both on the light-quantum hypothesis and

---

<sup>16</sup>For a detailed recent discussion of this aspect of Jordan's life and career, see (Hoffmann and Walker, 2007).

<sup>17</sup>For criticism see, e.g., (Smekal, 1926), (Heisenberg, 1931), (Born and Fuchs, 1939a), (Gonzalez and Wergeland, 1973), and (Bach, 1989).

<sup>18</sup>Jordan to Van der Waerden, December 1, 1961. Transcriptions of correspondence between Jordan and Van der Waerden in 1961–1962 can be found in the folder on Jordan in the *Archive for History of Quantum Physics*, cited hereafter as AHQP (Kuhn *et al.*, 1967). Van der Waerden relied heavily on this correspondence in editing his well-known anthology (Van der Waerden, 1968).

<sup>19</sup>Jordan to Van der Waerden, April 10, 1962 (AHQP), our emphasis. In view of the first sentence, it is not surprising that Ch. 4 of (Born and Jordan, 1925), "comments on electrodynamics," was left out of (Van der Waerden, 1968).



on the new matrix mechanics. In his dissertation, supervised by Born and published as (Jordan, 1924), he had criticized the argument for ascribing momentum to light quanta in (Einstein, 1917). He had “renounced this heresy”<sup>20</sup> after Einstein (1925) published a brief rejoinder. In another paper, Jordan (1925) showed that he was well versed in the latest statistical arguments concerning light quanta. And in late 1925, Jordan gave Born a manuscript in which he essentially proposed what is now known as Fermi-Dirac statistics. Unfortunately, the manuscript ended up at the bottom of a suitcase that Born took with him to the United States and did not resurface until Born returned from his trip, at which point Jordan had been scooped (Schroer, 2007, p. 49). In addition to his work in quantum statistics, Jordan was one of the founding fathers of matrix mechanics. The *Dreimännerarbeit* is the sequel to (Born and Jordan, 1925), which greatly clarified the theory proposed in Heisenberg’s *Umdeutung* paper. Unfortunately for Jordan, few if any physicists at the time were primed for his sophisticated combination of these two contentious lines of research—the statistics of light quanta and matrix mechanics—in his derivation of Einstein’s fluctuation formula.

### 10.3.2 The Reactions of Heisenberg and Born to Jordan’s Result

Even Jordan’s co-authors experienced great difficulty understanding his reasoning and entertained serious doubts about its validity. In the letter cited in note 18, Jordan wrote that “my reduction of light quanta to quantum mechanics was considered misguided [*abwegig*] by Born and Heisenberg for a considerable period of time.” In the letter to Van der Waerden cited in note 19, Jordan, after reiterating that these fluctuation considerations were “completely mine” (*ganz von mir*), elaborated on the resistance he encountered from his co-authors

Later, Heisenberg in fact explicitly questioned whether this application I had made of quantum mechanics to a system of *infinitely many degrees of freedom* was correct. It is true that Born did not second Heisenberg’s opinion at the time that it was wrong, but he did not explicitly reject Heisenberg’s negative verdict either.<sup>21</sup>

Jordan’s recollections fit with statements his co-authors made at various times.

A few weeks before the *Dreimännerarbeit* was submitted, Heisenberg wrote to Wolfgang Pauli: “Jordan claims that the interference calculations come out right, both the classical [wave] and the Einsteinian [particle] terms . . . I am a little unhappy about it, because I do not understand enough statistics to judge whether it makes sense; but I cannot criticize it either, because the problem itself and the calculations look meaningful to me.”<sup>22</sup> By 1929, Heisenberg had warmed to Jordan’s fluctuation calculations and he included them in his book based on lectures that year at the University of Chicago (Heisenberg, 1930, Ch. V, sec. 7).<sup>23</sup> On the face of it, Heisenberg (1931) lost faith again

<sup>20</sup>P. 13 of the transcript of session 2 of Thomas S. Kuhn’s interview with Jordan in June 1963 for the AHQP. For further discussion of (Jordan, 1924, 1925), see session 1, pp. 10–11, 15, and session 2, pp. 16–17 of the interview. For discussion of the section on fluctuations in the *Dreimännerarbeit*, including Jordan’s views of the work by Bothe (1923, 1924), see session 3, pp. 8–9.

<sup>21</sup>Jordan to Van der Waerden, April 10, 1962 (AHQP).

<sup>22</sup>Heisenberg to Pauli, October 23, 1925 (Pauli, 1979, p. 252), quoted (in slightly different translations) and discussed in (Darrigol, 1986, p. 220) and in (Mehra and Rechenberg, 1982–2001, Vol. 3, p. 149).

<sup>23</sup>We already quoted Heisenberg’s conclusion in the introduction.

the following year, when he showed that the mean square energy fluctuation diverges *if we include all possible frequencies*, even in a model that avoids the zero-point energy of the harmonic oscillators of the model used in the *Dreimännerarbeit*. As we shall see in sec. 10.4, however, Jordan clearly intended to calculate the mean square energy fluctuation *in a narrow frequency range*, even though his notation in various places suggests otherwise. In that case, the result is perfectly finite, regardless of whether we consider a model with or without zero-point energy. It is true that the mean square energy fluctuation as calculated by Jordan diverges when integrated over all frequencies. As Heisenberg showed in his 1931 paper, however, this is essentially an artifact of the idealization that the subvolume for which the energy fluctuations are computed has sharp edges (which necessarily excite arbitrarily high frequency modes). If the edges are smoothed out, the mean square energy fluctuation remains finite even when integrated over all frequencies.<sup>24</sup>

Jordan included his fluctuation argument in (Born and Jordan, 1930, sec. 73, pp. 392–400), a book on matrix mechanics. By the early 1930s, anyone who cared to know must have known that Jordan was responsible for this part of the *Dreimännerarbeit*. This can be inferred, for instance, from Pauli's scathing review of Born and Jordan's book. The reviewer wearily informs his readers that the authors once again trot out the "trains of thought about fluctuation phenomena, which one of the authors (P. Jordan) has already taken occasion to present several times before" (Pauli, 1930). These considerations can indeed be found in (Jordan, 1927b, p. 642; Jordan, 1928, pp. 192–196). They also form the starting point of a review of the current state of quantum electrodynamics at a conference in Charkow the following year (Jordan, 1929, pp. 700–702). We shall quote from these texts below.

That these fluctuation considerations make yet another appearance in (Born and Jordan, 1930) would seem to indicate Born's (belated) approval of Jordan's argument. In the late 1930s, however, in a paper written in exile in Edinburgh with his assistant Klaus Fuchs,<sup>25</sup> Born sharply criticizes Jordan's argument as well as Heisenberg's 1931 amendment to it. He goes as far as dismissing a central step in the argument in the *Dreimännerarbeit* as "quite incomprehensible reasoning,"<sup>26</sup> offering as his only excuse for signing off on this part of the paper "the enormous stress under which we worked in those exciting first days of quantum mechanics" (Born and Fuchs, 1939a, p. 263).

Born conveniently forgets to mention that he had signed his name to the same argument in the 1930 book. Stress had been a factor during the writing of that book as well. In the fall of 1930, still smarting from Pauli's sarcastic review of the book, Born wrote to Sommerfeld, Pauli's teacher:

[B]ecause I think very highly of Pauli's accomplishments, I am sorry that our personal relationship is not particularly good. You will probably have realized that on the basis of his criticism of [Born and Jordan, 1930] . . . I know full well that the book has major weaknesses, which are due in part to the fact that it was started too early and in part to the fact that I fell ill during

---

<sup>24</sup>See the discussion following Eq. (10.53) in sec. 10.4.2 for further details on Heisenberg's objection and its resolution.

<sup>25</sup>For Born's reaction to Fuchs's later arrest as a Soviet spy, see (Born, 1978, p. 288).

<sup>26</sup>In our reconstruction of Jordan's argument in sec. 10.4, we shall identify the step that Born and Fuchs found so objectionable (see note 68).

the work, a collapse from which unfortunately I still have not fully recovered. But from Pauli's side the nastiness of the attack has other grounds, which are not very pretty.<sup>27</sup>

Born then explains how he had originally asked Pauli to collaborate with him on the development of matrix mechanics and how he had only turned to Jordan after Pauli had turned him down (cf. Born, 1978, pp. 218–219). Ever since, Born continues, Pauli “has had a towering rage against Göttingen and has wasted no opportunity to vent it through mean-spirited comments” (Born to Sommerfeld, October 1, 1930). Born eventually came to agree with the substance of Pauli's criticism of his book with Jordan. In his memoirs, in a chapter written in the early 1960s (Born, 1978, p. 225), Born is very dismissive of the book and concedes that the authors' self-imposed restriction to matrix methods was a “blunder” for which they had rightfully been excoriated by Pauli. In his memoirs, Born's ire is directed not at Pauli but at Jordan, whom he blames for the Göttingen parochialism—or “local patriotism,” as he calls it—that led them to use matrix methods only (ibid., p. 230). It is possible that Born had already arrived at this assessment when he attacked Jordan's fluctuation considerations in his paper with Fuchs.

Whatever the case may be, a few months after the publication of their paper, Born and Fuchs (1939b) had to issue a “correction.” Pauli's assistant Markus E. Fierz had alerted them to a serious error in their calculations. The resulting two-page “correction” amounts to a wholesale retraction of the original paper. The authors explicitly withdraw their criticism of (Heisenberg, 1931) but do not extend the same courtesy to Jordan. This same pattern returns in Born's memoirs, in another chapter dating from the early 1960s, where Born writes that he and Fuchs “worked on the fluctuations in the black-body radiation but discovered later that Heisenberg had done the same, and better” (Born, 1978, p. 285). We find it hard to suppress the thought that, starting sometime in the 1930s, Born's perception of Jordan and Jordan's work became colored—and who can blame him?—by his former student's manifest Nazi sympathies.

### 10.3.3 Jordan's Result as an Argument for Field Quantization

As Jordan emphasized, both in the late 1920s and in reflecting on this period later, behind the initial resistance of Born and Heisenberg to his fluctuation calculation was a more general resistance to the notion of quantizing the electromagnetic field. As he told Kuhn: “The idea that from the wave field, i.e., from the electromagnetic field, one had to take another step to quantum mechanics struck many physicists back then as too revolutionary, or too artificial, or too complicated, and they would rather not believe it.”<sup>28</sup> The passage from a letter from Jordan to Van der Waerden (see note 21) that we quoted above already hints at this and it is made more explicit as the letter continues:

I remember that, to the extent that they took notice of these issues at all, other theorists in Göttingen [i.e., besides Born and Heisenberg], [Yakov] Frenkel for instance, considered my opinion, expressed often in conversation, that the electromagnetic field and the Schrödinger field had to be quantized ... as a somewhat fanciful exaggeration or as lunacy.<sup>29</sup> This changed only

<sup>27</sup>Born to Sommerfeld, October 1, 1930, quoted in Von Meyenn, 2007, pp. 45–47.

<sup>28</sup>AHQP interview with Jordan, session 3, p. 8.

<sup>29</sup>“... eine etwas phantastische Uebertreibung oder Verrücktheit.”

when Dirac [1927] also quantized both the electromagnetic field and the field of matter-waves. I still remember how Born, who had been the first to receive an offprint of the relevant paper of Dirac, showed it to me and initially looked at it shaking his head. When I then pointed out to him that I had been preaching the same idea all along ever since our *Dreimännerarbeit*, he first acted surprised but then agreed.<sup>30</sup> Heisenberg then also set aside his temporary skepticism, though it was not until considerably later that he himself started to work toward a quantum theory of fields (or “quantum electrodynamics”) in the paper he then published with Pauli,<sup>31</sup> which followed up on my three joint papers with Pauli, [Oskar] Klein, and [Eugene] Wigner.<sup>32,33</sup>

These and other publications of the late 1920s make Jordan one of the pioneers of quantum field theory. In his AHQP interview (session 3, p. 9), Jordan told Kuhn the same story he told Van der Waerden. Kuhn asked him in this context who had coined the phrase “second quantization.” Jordan told him he had (*ibid.*). A version of the story he told Van der Waerden and Kuhn in the early 1960s can already be found in a letter to Born of the late 1940s:

It has always saddened me somehow that the attack on the light-quantum problem already contained in our *Dreimännerarbeit* was rejected by everyone for so long (I vividly remember how Frenkel, despite his very friendly disposition toward me, regarded the quantization of the electromagnetic field as a mild form of insanity<sup>34</sup>) until Dirac took up the idea *from which point onward he was the only one cited in this connection*.<sup>35</sup>

Given the resentment one senses in the italicized clause, there is some irony in how Jordan segues into another version of the same story in the volume in honor of Dirac's 70th birthday:

*I have been extremely thankful to Dirac in another connection.* My idea that the solution of the vexing problem of Einstein's light quanta might be given by applying quantum mechanics to the Maxwell field itself, aroused the doubt, scepticism, and criticism of several good friends. But one day when I visited Born, he was reading a new publication of Dirac, and he said: ‘Look here, what Mr. Dirac does now. He assumes the eigenfunctions of a particle to be non-commutative observables again.’ I said: ‘Naturally.’ And Born said: ‘How can you say “naturally”?’ I said: ‘Yes, that is, as I have asserted repeatedly, the method which leads from the one-particle problem to the many-body problem in the case of Bose statistics’ (Jordan, 1973, p. 297; our emphasis).

---

<sup>30</sup>Jordan's text can be read as saying that Born agreed that Jordan had indeed been championing the same idea, but what he meant, presumably, is that Dirac's paper convinced Born of the merit of the idea.

<sup>31</sup>(Heisenberg and Pauli, 1929, 1930)

<sup>32</sup>(Jordan and Pauli, 1928; Jordan and Klein, 1927; Jordan and Wigner, 1928).

<sup>33</sup>Jordan to Van der Waerden, April 10, 1962 (AHQP).

<sup>34</sup>“... eine Art leichtes Irresein” [sic].

<sup>35</sup>Jordan to Born, July 3, 1948 (AHQP), our emphasis.

Since this was a conference honoring Dirac, other speakers can be forgiven for declaring Dirac to be the founding father of quantum field theory. Rudolf Peierls (1973, p. 370) set the tone in his talk on the development of quantum field theory and Julian Schwinger (1973, p. 414) followed suit in his report on quantum electrodynamics the next day. Gregor Wentzel chaired this session and the conference proceedings also contain a reprint of his review of quantum field theory for the Pauli memorial volume, which prominently mentions the *Dreimännerarbeit* and lists the early papers of Jordan and his collaborators in its bibliography (Wentzel, 1960, p. 49 and pp. 74–75). Neither Wentzel nor Jordan said anything in the discussions following the talks by Peierls and Schwinger. One wonders whether these celebratory distortions of history induced Jordan to submit his reminiscences of the early years of quantum mechanics to the conference proceedings instead of the musings on the expansion of the earth to which he had treated his colleagues at the conference itself.

More recent histories of quantum field theory—(Weinberg, 1977, pp. 19–20) but especially (Darrigol, 1986) and, drawing on Darrigol’s work, (Miller, 1994) and (Schweber, 1994)—do full justice to Jordan’s contributions.<sup>36</sup> To understand the negative reactions of his co-authors and contemporaries to his derivation of the fluctuation formula it is important to keep in mind that Jordan was virtually alone at first in recognizing the need for the extension of quantum theory to fields.

#### 10.3.4 The 1926 Smekal Interlude

What is suppressed in Jordan’s later recollections is that in 1926 he himself started to have second thoughts about second quantization and that (Dirac, 1927) also seems to have been important in dispelling his own doubts.<sup>37</sup> In April 1926, Adolf Smekal published a paper criticizing the fluctuation calculations in the *Dreimännerarbeit*. Smekal argued that, when calculating energy fluctuations in radiation, one should take into account the interaction with matter emitting and absorbing the radiation. Without such interaction, he insisted, the radiation would not reach its equilibrium black-body frequency distribution and would not be detectable so that *a fortiori* fluctuations in its energy would not be observable.

With the first of these two objections, Smekal put his finger on a step that is missing

---

<sup>36</sup>See also (Ehlers, 2007) and (Schroer, 2007), specifically on Jordan, as well as (Weinberg, 1995, sec. 1.2, pp. 15–31). It is difficult to gauge both how well-known and how well-understood these calculations have been in the physics community since their publication in 1926. One data point is provided by (Milonni, 1981, 1984). In 1981, this author derived a formula for energy fluctuations in a box of black-body radiation (*not* a subvolume of this box) that has the form of Einstein’s 1909 fluctuation formula. He interprets the two terms in his fluctuation formula “in terms of the fundamental processes of spontaneous and stimulated emission, and absorption” and writes that “[t]his interpretation seems obvious in retrospect but has not, to the author’s knowledge, been discussed previously” (ibid.). He does not mention the *Dreimännerarbeit*. In a paper on wave-particle duality three years later in a volume in honor of Louis de Broglie’s 90th birthday, Milonni (1984, pp. 39–41) does mention the fluctuation calculations in the *Dreimännerarbeit*, though he has clearly missed that these calculations, like Einstein’s, pertain to a *subvolume* and seems to be under the impression that they are equivalent to the calculations in (Milonni, 1981). He acknowledges that, when he wrote this 1981 paper, he “was not aware that the Born-Heisenberg-Jordan paper contained a discussion of the fluctuation formula” (Milonni, 1984, p. 62, note 27). Neither were the editors and referees of *American Journal of Physics* it seems.

<sup>37</sup>This interlude is also discussed in (Darrigol, 1986, pp. 222–225).

both in H. A. Lorentz's (1916) derivation of the classical formula for the mean square energy fluctuation in black-body radiation, and in Jordan's derivation of its quantum counterpart in the simple model of a string. To derive a formula for *thermal* fluctuations, one needs to consider a thermal ensemble of states. Both Lorentz and Jordan, however, only considered individual states and failed to make the transition to an ensemble of states. A clear indication of the incompleteness of their derivations is that the temperature does not appear anywhere. Smekal is quite right to insist that we consider the system, be it black-body radiation or oscillations in a string, in contact with an external heat bath. This does not mean, however, that the interaction with matter needs to be analyzed in any detail. We can calculate the thermal fluctuations simply assuming that the system has somehow thermalized through interaction with matter. It should also be emphasized that the fluctuations in a small subvolume that Lorentz and Jordan were interested in do not come from the exchange of energy between radiation and matter but from radiation energy entering and leaving the subvolume. Smekal's second objection—that interaction with matter is needed to detect energy fluctuations in radiation—seems to have gained considerable traction with the authors of the *Dreimännerarbeit*, as one would expect given their Machian-positivist leanings.

In response to Smekal's criticism of their paper, the authors retreated to the position that their calculation was certainly valid for sound waves in a solid<sup>38</sup> and that it was still an open question whether it also applied to electromagnetic radiation. This is clear from a paper by Heisenberg (1926, p. 501, note 2) on fluctuation phenomena in crystal lattices and from a letter he simultaneously sent to Born, Jordan, and Smekal. As he told these three correspondents:

Our treatment [i.e., in the *Dreimännerarbeit*] of fluctuation phenomena is undoubtedly applicable to the crystal lattice ... The question whether this computation of fluctuations can also be applied to a radiation cavity can, as Mr. Smekal emphasizes, not be decided at the moment, as a quantum mechanics of electro-dynamical processes has not been found yet. Because of the formal analogy between the two problems (crystal lattice–cavity) I am personally inclined to believe in this applicability, but for now this is just a matter of taste.<sup>39</sup>

A more definite stance would have to await the quantum-mechanical treatment of a full interacting system of radiation and matter. Dirac's paper provided such a treatment.

The retreat triggered by (Smekal, 1926) and the renewed advance after (Dirac, 1927) left some traces in Jordan's writings of this period. Immediately after the discussion of his fluctuation considerations in his semi-popular history of the light-quantum hypothesis, we read:

For light itself one can look upon the following thesis as the fundamental result of the investigation of Born, Heisenberg, and Jordan, namely that (as demanded by Pauli) a new *field concept* must be developed in which one applies the concepts of quantum mechanics to the oscillating field. But

---

<sup>38</sup>In his lecture on specific heats at the first Solvay conference in 1911, Einstein (1914, p. 342) had already made it clear that these fluctuation considerations also apply to solids (Bach, 1989, p. 180).

<sup>39</sup>Heisenberg to Born, Jordan, and Smekal, October 29, 1926 (AHQP).

this thesis has in a sense shared the fate of the [fluctuation] considerations by Einstein, the elucidation of which served as its justification: for a long time—even among proponents of quantum mechanics—one either suspended judgement or rejected the thesis. It was accepted only when Dirac showed a year later that Einstein’s [1917] laws for emission and absorption for atoms in a radiation field also follow necessarily and exactly from this picture [of quantized fields] (Jordan, 1928, pp. 195–196).

In a footnote appended to the next-to-last sentence, Jordan acknowledges that “this general rejection” of field quantization had caused him to doubt it himself “for a while” and that these doubts had found their way into his two-part overview of recent developments in quantum mechanics (Jordan, 1927a,b). In his presentation of his fluctuation considerations in the second part, Jordan (1927b, pp. 642–643) indeed accepted Heisenberg’s criticism (cf. note 21) that it is unclear whether quantum mechanics as it stands applies to systems with an infinite number of degrees of freedom and, again following Heisenberg’s lead, retreated to the claim that the analysis certainly holds for a lattice with a finite number of particles. In the *Dreimännerarbeit*, the authors still confidently asserted that the same considerations that apply to a finite crystal lattice “also apply if we go over to the limiting case of a system with infinitely many degrees of freedom and for instance consider the vibrations of an elastic body idealized to a continuum or finally of an electromagnetic cavity” (p. 375). In a note added in proof to his paper the following year, Jordan (1927b, p. 643) announced with obvious relief that Dirac’s forthcoming paper completely vindicates the original generalization from a lattice to radiation.

### 10.3.5 Jordan’s Result As Evidence for Matrix Mechanics

The ambivalence of Born and Heisenberg about Jordan’s fluctuation considerations is reflected in the use that is made of Jordan’s result in the *Dreimännerarbeit*. Rather than hailing it as a seminal breakthrough in understanding the wave-particle duality of light, the authors make it subordinate to the overall aim of promoting matrix mechanics. As they announce at the end of the introduction, the derivation of the fluctuation formula “may well be regarded as significant evidence in favour of the quantum mechanics put forward here” (p. 325). After presenting the result, they comment:

If one bears in mind that the question considered here is actually somewhat remote from the problems whose investigation led to the growth of quantum mechanics, the result . . . can be regarded as particularly encouraging for the further development of the theory (p. 385).

The one other accomplishment the authors explicitly identify as providing “a strong argument in favour of the theory” is their derivation of the Kramers dispersion formula, “otherwise obtained only on the basis of correspondence considerations” (p. 333). Since the new theory grew directly out of such considerations (Duncan and Janssen, 2007), it is not terribly surprising that it correctly reproduces this formula. The recovery of the Einstein fluctuation formula, which played no role in the construction of the theory, constitutes much more striking evidence.

Moreover, as the authors themselves emphasize, the way in which the theory reproduces the fluctuation formula is a particularly instructive illustration of the basic idea

of *Umdeutung*. Before going into the details of the calculations, the authors already express the hope “that the modified kinematics which forms an inherent feature of the theory proposed here would yield the correct value for the interference fluctuations” (p. 377). In the next-to-last paragraph of the paper, they make sure the reader appreciates that this hope has now been fulfilled:

The reasons leading to the appearance [in the formula for the mean square energy fluctuation] of a term which is not provided by the classical theory are obviously closely connected with the reasons for [the] occurrence of a zero-point energy. The basic difference between the theory proposed here and that used hitherto in both instances lies in the characteristic kinematics and not in a disparity of the mechanical laws. One could indeed perceive one of the most evident examples of the difference between quantum-theoretical kinematics and that existing hitherto on examining [the quantum fluctuation formula], which actually involves no mechanical principles whatsoever (p. 385).

With the exception of the final clause, which is best set aside as a rhetorical flourish, the authors' point is well taken. In the spirit of Heisenberg's groundbreaking paper, “Quantum-theoretical re-interpretation of kinematic and mechanical relations,” the fluctuation formula, the Kramers dispersion formula, and other results are obtained not through a change of the dynamical laws (the  $q$ 's and  $p$ 's for the oscillators representing the modes of the field satisfy the usual laws of Newtonian mechanics) but through a change of the kinematics (the nature of the  $q$ 's and  $p$ 's is changed). In this particular case, this means that, although the wave equation for the string—used here as a proxy for Maxwell's equations—is taken over intact from the classical theory, the displacement of the continuous string from its equilibrium state and the time derivatives of that displacement are no longer given by an infinite set of numbers but rather by an infinite set of infinite-dimensional matrices.

The Hamiltonian for a vibrating string decomposes, both classically and quantum-mechanically, into a sum over infinitely many uncoupled harmonic oscillators. The occurrence of a particle-like term in the quantum formula for the mean square energy fluctuation in a segment of the string is a direct consequence of the zero-point energy of these oscillators. The zero-point energy of the harmonic oscillator had already been derived in the *Umdeutung* paper (Heisenberg, 1925, pp. 271–272; see also Born and Jordan, 1925, pp. 297–300). Stachel (1986, p. 379), in a classic paper on Einstein and quantum physics, correctly identifies the zero-point energy as the key element in Jordan's derivation of the fluctuation formula, but does not mention that the zero-point energy itself is traced to the central new feature of the new theory, the *Umdeutung* of position and momentum as matrices subject to a quantum commutation relation. Without this additional piece of information, it looks as if Jordan obtained his result simply by sleight of hand. Kojevnikov (1990, p. 212) does mention that the zero-point energy is itself a consequence of the new theory, though the point could have done with a little more emphasis. Darrigol (1986, p. 222), in his brief characterization of Jordan's calculation, stresses the role of non-commutativity and does not explicitly mention the zero-point energy at all.<sup>40</sup>

---

<sup>40</sup> Bach (1989, p. 199) acknowledges that “sometimes it is pointed out that the cause of the occurrence of the two terms [in the fluctuation formula] lies in the non-commutativity of the observables of the



In 1926, Heisenberg, in the letter from which we already quoted in sec. 10.3.4, made it clear that the fluctuation calculations were important to him only insofar as they provided evidence for matrix mechanics and, by this time, against wave mechanics:

For the crystal lattice the quantum-mechanical treatment [of fluctuations] undoubtedly means essential progress. This progress is not that one has found the mean square fluctuation; that one already had earlier and is obvious on the basis of general thermodynamical considerations if one introduces quantum jumps. The progress, in fact, is that quantum mechanics allows for the calculation of these fluctuations without explicit consideration of quantum jumps on the basis of relations between  $q$ ,  $q'$  etc. This amounts to a strong argument for the claim that quantum-mechanical matrices are the appropriate means for representing discontinuities such as quantum jumps (something that does not become equally clear in the wave-mechanical way of writing things). The calculation of our *Dreimännerarbeit* thus provided an element of support for the correctness of quantum mechanics.<sup>41</sup>

Now that the calculation had served that purpose, Heisenberg clearly preferred to leave it behind and move on.<sup>42</sup> In fact, he closes his letter reminding his correspondents that “there are so many beautiful things in quantum theory at the moment that it would be a shame if no consensus could be reached on a detail like this” (*eine solche Einzelheit*; *ibid.*).

### 10.3.6 Jordan’s Result as Solving the Riddle of the Wave-Particle Duality of Light

For Jordan, the value of the fluctuation result as solving the riddle of the wave-particle duality of light was obviously much higher than for Heisenberg. Still, Jordan also had a tendency to make it subservient to a larger cause, albeit field quantization rather than matrix mechanics. We already quoted Jordan (1928, pp. 195–196) saying that the fundamental importance of the result was that it brought out the need to quantize fields. In this same article, however, as in various subsequent publications, Jordan also did full justice to the importance of the result as having resolved the conundrum of the wave-particle duality of light. In his history of the light-quantum hypothesis, he wrote:

[I]t turned out to be superfluous to explicitly adopt the light-quantum hypothesis: We explicitly stuck to the wave theory of light and only changed the kinematics of cavity waves quantum-mechanically. From this, however, the

---

quantum theory,” but claims that this is mistaken since the observables relevant to the fluctuation problem supposedly form an Abelian subalgebra (*ibid.*, pp. 199, 202). This claim is simply false. The relevant observables, the operator for the energy of the whole system and the operator for the energy in part of the system in a narrow frequency range, do not commute (see sec. 10.4.2, the discussion following eq. (10.59)).

<sup>41</sup>Heisenberg to Born, Jordan, and Smekal, October 29, 1926 (AHQP).

<sup>42</sup>In the same letter, Heisenberg claimed that he only reluctantly agreed to the publication of the section on fluctuation phenomena of the *Dreimännerarbeit*: “I wanted to give up on publishing our *Dreimännernote*, because all polemics are abhorrent to me in the bottom of my soul [*weil mir jede Polemik im Grund meiner Seele völlig zuwider ist*] and because I no longer saw any point worth fighting for.”

characteristic light-quantum effects emerged automatically as a consequence . . . This is a whole new turn in the light-quantum problem. It is not necessary to include the picture [*Vorstellung*] of light quanta among the assumptions of the theory. One can—and this seems to be the natural way to proceed—start from the wave picture. If one formulates this with the concepts of quantum mechanics, then the characteristic light-quantum effects emerge as necessary consequences from the general laws [*Gesetzmäßigkeiten*] of quantum theory (Jordan, 1928, p. 195).

As Jordan undoubtedly realized, “the characteristic light-quantum effects” referred to in this passage do not include those that involve interaction between the electromagnetic field and matter, such as the photoelectric effect or the Compton effect. His argument only applies to free radiation.<sup>43</sup> As such, however, it does explain why the Einstein fluctuation formula contains both a particle and a wave term and why light quanta are subject to Bose’s odd new statistics. That the latter also speaks in favor of Jordan’s approach is explicitly mentioned in the *Dreimännerarbeit* (pp. 376–379), in (Jordan, 1928, p. 182), and, in more detail, in Jordan’s textbook on quantum mechanics (Jordan, 1936, p. 220).<sup>44</sup> The connection with Bose statistics is not mentioned in (Jordan, 1929), his contribution to the proceedings of the Charkow conference on unified field theory and quantum mechanics. That is probably because the paper is not about quantum statistics but about quantum field theory. As such it provides a prime example of Jordan using his fluctuation result as a means to an end (i.e., the promotion of field quantization), but it also contains a particularly crisp statement of the value of the result as the solution to the riddle of the wave-particle duality of light, complete with an uncharacteristically immodest assessment of its momentous character:

Einstein drew the conclusion that the wave theory would necessarily have to be replaced or at least supplemented by the corpuscular picture. With our findings [*Feststellungen*], however, the problem has taken a completely different turn. We see that it is not necessary after all to abandon or restrict the wave theory in favor of other models [*Modellvorstellungen*]; instead it just comes down to reformulating [*übertragen*] the wave theory in quantum mechanics. The fluctuation effects, which prove the presence of corpuscular light quanta in the radiation field, then arise automatically as consequences of the wave theory. The old and famous problem how one can understand waves and particles in radiation in a unified manner can thus in principle be considered as taken care of [*erledigt*] (Jordan, 1929, p. 702)

The strong confidence conveyed by that last sentence probably reflects that with (Dirac, 1927) the tide had decisively turned for Jordan’s pet project of quantizing fields. Jordan’s language in (Born and Jordan, 1930, pp. 398–399) is admittedly more subdued again, but that could be because he feared he would not get a more exuberant statement past his teacher and co-author. As is clear in hindsight (see sec. 10.3.2), Born was not paying

---

<sup>43</sup>As mentioned in sec. 10.3.4, Dirac (1927) first developed the theory for the interaction between the electromagnetic field and matter.

<sup>44</sup>For discussion of the connection to Bose statistics, see (Darrigol, 1986, p. 221). Darrigol quotes from a letter from Jordan to Erwin Schrödinger that can be dated to the summer of 1927, in which Jordan briefly reiterates this point (ibid., p. 224).

much attention and Jordan need not have worried, but Jordan probably did not know that in 1930. In any event, the language of the Charkow proceedings, including the triumphant last sentence, is recycled *verbatim* in (Jordan, 1936, p. 222).

None of these later texts ever drew anywhere near the attention accorded to the *Dreimännerarbeit*. Reading them *seriatim*, moreover, one can appreciate the complaint by Pauli (1930) to the effect that Jordan was starting to sound like a broken record (see sec. 10.3.2). Jordan did himself a disservice not only by agreeing to present his result merely as a piece of evidence for matrix mechanics in the *Dreimännerarbeit*, but also by trying to make up for that mistake too many times. That Jordan routinely pressed the result into service in his promotion of quantum field theory may also have hurt the recognition of its significance as solving the riddle of the wave-particle duality of light.

### 10.3.7 Einstein's Reaction to Jordan's Result

As the person responsible for the riddle, Einstein should have been especially interested in the solution Jordan claimed to have found. As Jordan told Van der Waerden: "Einstein was really the only physicist from whom I could expect the acknowledgment [*Feststellung*] that with this result a big problem in physics had really been brought to its solution. But, although he reacted very friendly and kindly, Einstein on his part was disinclined to consider matrix mechanics as trustworthy."<sup>45</sup> He told Kuhn the same thing: "One might have imagined that Einstein would have been pleased [with Jordan's result] but Einstein's attitude toward matrix mechanics was that he was having none of it" (AHQP interview with Jordan, session 3, p. 9).<sup>46</sup>

In late October 1925, as the *Dreimännerarbeit* was being completed, Jordan wrote to Einstein enclosing some notes on his fluctuation calculations.<sup>47</sup> Einstein's response has not been preserved (see note 8), but from Jordan's next letter a month and a half later, it can be inferred that Einstein objected to the use of the zero-point energy in the calculation. In his defense, Jordan wrote:

My opinion of the zero-point energy of the cavity is roughly that it is really only a formal calculational quantity without direct physical meaning; only the thermal energy referred to  $T = 0$  is physically definable. The fluctuations, which formally have been calculated as the mean square fluctuation of thermal energy + zero-point energy, are, of course, *identical with the fluctuations of the thermal energy*.<sup>48</sup>

---

<sup>45</sup>Jordan to Van der Waerden, December 1, 1961 (AHQP). As the reference to Einstein's friendliness suggests, politics did not play a role in Einstein's negative reaction.

<sup>46</sup>In a letter to Ehrenfest of September 30, 1925, Einstein ironically referred to Heisenberg's "large quantum egg" (Fölsing, 1997, p. 566).

<sup>47</sup>Jordan to Einstein, October 29, 1925 (AE 13-473), dated by a reference to Born's departure for the United States the day before. The enclosed notes, it seems, are no longer extant. In the letter, Jordan announces that his paper with Born and Heisenberg will be ready in "8 to 14 days." The *Dreimännerarbeit* was received by *Zeitschrift für Physik* on November 16, 1925.

<sup>48</sup>Jordan to Einstein, December 15, 1925 (AE 13-474). Jordan inquires whether Einstein had meanwhile received page proofs of the *Dreimännerarbeit*, suggesting that Einstein only had Jordan's notes to go on at this point. Jordan also writes that he is planning to develop "a systematic matrix theory of the electromagnetic field" based on the formalism developed by Born and Norbert Wiener. In view of Jordan's later assessment of the importance of his fluctuation result (see the passages quoted in sec. 10.3.6), it is interesting note that he wrote to Einstein that such a theory would "still remain far

The answer did not satisfy Einstein. He continued to raise objections to the fluctuation calculations, first in letters to Heisenberg<sup>49</sup> and Ehrenfest,<sup>50</sup> then in a postcard to Jordan. This is the only contribution from Einstein to the correspondence with Jordan that has survived. In it, Einstein objects—to use the terminology that Jordan himself later introduced (see sec. 10.2)—that matrix mechanics can only reproduce his second fluctuation formula, not the first:

The thing with the fluctuations is fishy [*faul*]. One can indeed calculate the average magnitude of fluctuations with the zero-point term  $\frac{1}{2}h\nu$ , but not the probability of a very large fluctuation. For weak (Wien) radiation, the probability, for instance, that all radiation [in a narrow frequency range around  $\nu$ ] is found in a subvolume  $V$  of the total volume  $V_0$  is  $W = (V/V_0)^{E/h\nu}$ . This can evidently not be explained with the zero-point term although the expression is secure [*gesichert*] on thermodynamical grounds.<sup>51</sup>

Presumably, Einstein's problem with the zero-point energy was that, if the energy of each quantum of frequency  $\nu$  were  $\frac{3}{2}h\nu$  rather than  $h\nu$ , the exponent in the expression for  $W$  can no longer be interpreted as the number of light quanta  $N$  and black-body radiation in the Wien regime would no longer behave as an ideal gas of  $N$  particles. The zero-point energy, however, does not come into play here, since the energy  $E$  in the exponent of Einstein's formula is a thermal average of the excitation energy, the difference between the full energy and the zero-point energy, which Jordan in the quotation above called the "thermal energy."<sup>52</sup>

In his response, Jordan does not return to the issue of the zero-point energy but focuses on the question whether matrix mechanics allows one to calculate the probability of specific fluctuations.<sup>53</sup> He explains that the only way to do this in the theory as it stands is through expansion of such probabilities as power series in the mean square and higher-order fluctuations  $((E - \bar{E})^2, (E - \bar{E})^4, \text{etc.}; \text{cf. Jordan, 1928, p. 194})$ . In October 1927, Jordan revisited both objections in another letter to Einstein.<sup>54</sup> He conceded that the treatment of zero-point energy in the theory remained unsatisfactory and referred Einstein to comments on the issue in a paper he had in the works (Jordan and Pauli, 1928). However, the problem of arbitrary fluctuations, Jordan claimed, had been completely resolved. Referring to work soon to be published as (Jordan, 1927c), received by *Zeitschrift für Physik* on October 11, 1927, he wrote:

---

removed from the ideal ... a more profound light-quantum theory, in which a continuous world and continuous quantities no longer occur at all."

<sup>49</sup>This can be inferred from a letter from Jordan to Einstein that can be dated to February 1926 (AE 13-475), in which Jordan mentions that he has read a letter from Einstein to Heisenberg.

<sup>50</sup>Einstein to Ehrenfest, February 12, 1926, quoted in (Kojevnikov, 1990, p. 212).

<sup>51</sup>Einstein to Jordan, March 6, 1926 (AHQP), quoted, for instance, in (Mehra and Rechenberg, 1982–2001, Vol. 3, p. 156). In a postscript Einstein added somewhat disingenuously: "Other than that, however, I am greatly impressed with matrix theory." The objections raised in this postcard can also be found in the letter to Ehrenfest cited in the preceding note.

<sup>52</sup>This term is also used in the *Dreimännerarbeit* (p. 377, p. 384). As we shall argue in sec. 10.4.2, this terminology is somewhat misleading (see the discussion following Eq. (10.56)).

<sup>53</sup>Jordan to Einstein (AE 13-472), undated but probably written shortly after Einstein's postcard of March 6, 1926.

<sup>54</sup>This letter (AE 13-478) was dated on the basis of a reference to page proofs of (Jordan and Klein, 1927), which was received by *Zeitschrift für Physik* on October 4, 1927.

Following the latest papers by Dirac, I have recently studied somewhat more closely the correspondence between a quantized wave field and a system of corpuscular quanta. This closer examination reveals such a perfect internal equivalence between these two systems that one can make the following claim: When, without explicitly appealing to the corpuscular representation, one simply quantizes the oscillations of the radiation field (like I did earlier for the vibrating string), one arrives *in all respects* at the same results as when one proceeds on the basis of the corpuscular representation . . . One then sees immediately that every lawlike regularity understandable on the basis of the corpuscular representation (such as, in particular, your formula  $W = (V/V_0)^{E/h\nu}$ ) is also a necessary consequence of the representation of quantized waves.<sup>55</sup>

Einstein's response, if there ever was any, has not been preserved. And Jordan never showed in detail how he could recover Einstein's first fluctuation formula. Of course, it is no condemnation of his derivation of the second fluctuation formula that he did not produce a derivation of the first.

Einstein never accepted Jordan's results and maintained to the end of his life that the puzzle of the wave-particle duality of light still had to be solved. As he told Michele Besso a few years before he died: "All these fifty years of conscious brooding have brought me no closer to the answer to the question "What are light quanta?" Nowadays every Tom, Dick, and Harry [*jeder Lump*] thinks he knows it, but he is mistaken."<sup>56</sup> Einstein scholars typically quote such pronouncements approvingly in recounting the story of the light-quantum hypothesis and the wave-particle duality of light.<sup>57</sup> Their message, it seems, is that, as wrong as Einstein turned out to be about other aspects of quantum mechanics, he was *right* about the wave-particle duality of light. In our estimation, he was just stubborn. Quantum electrodynamics provides a perfectly satisfactory solution to Einstein's 1909 riddle of the wave-particle duality of light. Jordan was the first to hit upon that solution. The problem of the infinite zero-point energy, to be sure, is still with us in the guise of the problem of the vacuum energy, but that is a different issue.<sup>58</sup> Recall, moreover, that Jordan avoided the problem of infinite zero-point energy altogether by deriving the mean square energy fluctuation in a finite frequency range.

---

<sup>55</sup>Jordan to Einstein, October 1927 (AE 13-478). A similar statement can be found in (Jordan, 1927c, pp. 772-774). This paper cites (Dirac, 1926, 1927). In (Born and Jordan, 1930, p. 399), the authors promise that it will be shown in a sequel to the book that a theory of quantized waves correctly reproduces Einstein's first fluctuation formula. Since (Born and Jordan, 1930) was itself the sequel to (Born, 1925), Pauli (1930) began his review by pointing out that "[t]his book is the second volume in a series in which goal and purpose of the *n*th volume is always made clear through the virtual existence of the (*n* + 1)th volume." The review helped ensure that, for *n* = 2, the (*n* + 1)th volume never saw the light of day.

<sup>56</sup>Einstein to Besso, December 12, 1951, quoted, for instance, in (Klein, 1979, p. 133, p. 138).

<sup>57</sup>See, e.g., (Stachel, 1986, pp. 379-380) and (Klein, 1970, pp. 38-39).

<sup>58</sup>For the free-field limit of quantum electrodynamics needed for the fluctuation calculations at issue here, a mathematically precise formulation is obtained by shifting the zero point of energy in the full Hamiltonian to remove the divergent zero-point energy contribution (which is the only divergence exhibited by a free field theory). Since such a shift clearly does not affect the dispersion in the energy, it also does not affect the mean square fluctuation in the energy in a subvolume and in a finite frequency interval.

### 10.3.8 Why Jordan's Result Has Not Become More Famous

In the course of our analysis in secs. 3.1–3.7, we identified several factors that help explain why Jordan's derivation of Einstein's fluctuation formula has not become part of the standard story of wave-particle duality. Before moving on to the actual calculations, we collect these factors here. First, there is the cloud of suspicion that has always surrounded the result. Then there is the tendency, most notably in the case of Heisenberg but also in the case of Jordan himself, to downplay the value of the result as resolving the conundrum of the wave-particle duality of light and to present it instead as an argument for either matrix mechanics or field quantization. This is reflected in the historical literature where Jordan's result has meanwhile found its proper place in histories of quantum field theory but is hardly ever mentioned in histories of the light-quantum hypothesis or wave-particle duality.

## 10.4 Reconstruction of and Commentary on Jordan's Derivation of Einstein's Fluctuation Formula

Jordan borrowed a simple model from Ehrenfest (1925, pp. 367–373) to analyze the problem of energy fluctuations in black-body radiation. He considered a string of length  $l$  fixed at both ends of constant elasticity and constant mass density. This can be seen as a one-dimensional analogue of an electromagnetic field forced to vanish at the conducting sides of a box. The wave equation for the string—the analogue of the free Maxwell equations for this simple model—is:

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0, \quad (10.4)$$

where  $u(x, t)$  is the displacement of the string at position  $x$  and time  $t$  and where the velocity of propagation is set equal to unity. The boundary conditions  $u(0, t) = u(l, t) = 0$  for all times  $t$  express that the string is fixed at both ends. The general solution of this problem can be written as a Fourier series (Ch. 4, Eqs. (41) and (41')):

$$u(x, t) = \sum_{k=1}^{\infty} q_k(t) \sin(\omega_k x), \quad (10.5)$$

with angular frequencies

$$\omega_k \equiv \frac{k\pi}{l}, \quad (10.6)$$

and Fourier coefficients (Ch. 4, Eq. (44))

$$q_k(t) = a_k \cos(\omega_k t + \varphi_k). \quad (10.7)$$

The Hamiltonian for the string is (Ch. 4, Eq. (42) [ $u^2$  should be  $\dot{u}^2$ ]):

$$H = \frac{1}{2} \int_0^l dx (\dot{u}^2 + u_x^2), \quad (10.8)$$

where the dot indicates a time derivative and the subscript  $x$  a partial derivative with respect to  $x$ . The terms  $\dot{u}^2$  and  $u_x^2$  are the analogues of the densities of the electric and

the magnetic field, respectively, in this simple model of black-body radiation. Inserting Eq. (10.5) for  $u(x, t)$  in Eq. (10.8), we find (Ch. 4, Eq. (41)):

$$H = \frac{1}{2} \int_0^l dx \sum_{j,k=1}^{\infty} (\dot{q}_j(t)\dot{q}_k(t) \sin(\omega_j x) \sin(\omega_k x) + \omega_j \omega_k q_j(t)q_k(t) \cos(\omega_j x) \cos(\omega_k x)). \quad (10.9)$$

The functions  $\{\sin(\omega_k x)\}_k$  in Eq. (10.5) are orthogonal on the interval  $(0, l)$ , i.e.,

$$\int_0^l dx \sin(\omega_j x) \sin(\omega_k x) = \frac{l}{2} \delta_{jk}. \quad (10.10)$$

The same is true for the functions  $\{\cos(\omega_k x)\}_k$ . It follows that the integral in Eq. (10.9) will only give contributions for  $j = k$  (as can be verified explicitly by substituting  $l$  for  $a$  in Eq. (10.18) below). The double sum thus turns into the single sum:

$$H = \sum_{j=1}^{\infty} \frac{l}{4} (\dot{q}_j^2(t) + \omega_j^2 q_j^2(t)) = \sum_{j=1}^{\infty} H_j. \quad (10.11)$$

With the help of Eqs. (10.6)–(10.7), we find that  $H_j = (l/4)a_j^2\omega_j^2 = j^2\pi^2 a_j^2/4l$ . It follows that the total energy in the string is finite as long as the amplitudes  $a_j$  fall off with  $j$  faster than  $j^{-3/2}$ .

Eq. (10.11) shows that the vibrating string can be replaced by an infinite number of uncoupled oscillators, one for every mode of the string. This shows that the distribution of the energy over the frequencies of these oscillators is constant in time. Since there is no coupling between the oscillators, there is no mechanism for transferring energy from one mode to another. The spatial distribution of the energy in a given frequency range over the length of the string, however, varies in time. We study the fluctuations of the energy in a narrow frequency range in a small segment of the string. The total energy in that frequency range will be constant but the fraction located in that small segment will fluctuate. Jordan derived an expression for the mean square energy fluctuation of this energy, first in classical theory, then in matrix mechanics.

### 10.4.1 Classical Calculation

Changing the upper boundary of the integral in Eq. (10.9) from  $l$  to  $a$  ( $a \ll l$ ) and restricting the sums over  $j$  to correspond to a narrow angular frequency range  $(\omega, \omega + \Delta\omega)$ , we find the instantaneous energy in that frequency range in a small segment  $(0, a) \subset (0, l)$  of the string. This quantity is simply called  $E$  in the paper (cf. Ch. 4, Eq. (43)). We add the subscript  $(a, \omega)$ :

$$E_{(a,\omega)}(t) = \frac{1}{2} \int_0^a dx \sum_{j,k} (\dot{q}_j(t)\dot{q}_k(t) \sin(\omega_j x) \sin(\omega_k x) + \omega_j \omega_k q_j(t)q_k(t) \cos(\omega_j x) \cos(\omega_k x)), \quad (10.12)$$

where the sums over  $j$  and  $k$  are restricted to the finite range of integers satisfying  $\omega < j(\pi/l) < \omega + \Delta\omega$  and  $\omega < k(\pi/l) < \omega + \Delta\omega$ . Unless we explicitly say that sums run

from 1 to  $\infty$ , *all* sums in what follows are restricted to this finite range. This restriction also appears to be in force in many summations in this section of the *Dreimännerarbeit* even though they are all *written* as infinite sums. The sums in Eqs. (43), (45), (46'), (46''), and (47) in the paper (pp. 381–382) should all be over this finite rather than over an infinite range of integers.

There are several clear indications in this section of the paper that the authors are in fact considering a small frequency range. The clearest statement is their description of the situation with black-body radiation which the string is supposed to represent:

If there is communication between a volume  $V$  and a very large volume such that waves which have *frequencies which lie within a small range  $\nu$  to  $\nu + d\nu$*  can pass unhindered from one to the other, whereas for all other waves the volumes remain detached, and if  $E$  be the energy of the waves with frequency  $\nu$  in  $V$ , then according to Einstein the mean square deviation ... can be calculated (p. 379, our emphasis).

Two pages later, in Eq. (43), the same symbol  $E$  is used for what we more explicitly write as  $E_{(a,\omega)}$ . Immediately below this equation it says in parentheses: “under the explicit assumption that all wavelengths *which come into consideration* are small with respect to  $a$ ” (p. 381, our emphasis).

The functions  $\{\sin(\omega_k x)\}_k$  and the functions  $\{\cos(\omega_k x)\}_k$  are not orthogonal on the interval  $(0, a)$ , so both terms with  $j = k$  and terms with  $j \neq k$  will contribute to the instantaneous energy  $E_{(a,\omega)}(t)$  in Eq. (10.12). First consider the ( $j = k$ ) terms. On the assumption that  $a$  is large enough for the integrals over  $\sin^2(\omega_j x)$  and  $\cos^2(\omega_j x)$  to be over many periods corresponding to  $\omega_j$ , these terms are given by:

$$E_{(a,\omega)}^{(j=k)}(t) \approx \frac{a}{4} \sum_j (\dot{q}_j^2(t) + \omega_j^2 q_j^2(t)) = \frac{a}{l} \sum_j H_j(t). \quad (10.13)$$

Since we are dealing with a system of uncoupled oscillators, the energy of the individual oscillators is constant. Since all terms  $H_j(t)$  are constant,  $E_{(a,\omega)}^{(j=k)}(t)$  is constant too and equal to its time average:<sup>59</sup>

$$E_{(a,\omega)}^{(j=k)}(t) = \overline{E_{(a,\omega)}^{(j=k)}(t)}. \quad (10.14)$$

Since the time averages  $\overline{\dot{q}_j(t)\dot{q}_k(t)}$  and  $\overline{q_j(t)q_k(t)}$  vanish for  $j \neq k$ , the ( $j \neq k$ ) terms in Eq. (10.12) do not contribute to its time average:

$$\overline{E_{(a,\omega)}^{(j \neq k)}(t)} = 0. \quad (10.15)$$

The time average of Eq. (10.12) is thus given by the ( $j = k$ ) terms:

$$E_{(a,\omega)}^{(j=k)}(t) = \overline{E_{(a,\omega)}^{(j=k)}(t)}. \quad (10.16)$$

Combining Eqs. (10.13) and (10.16), we see that the time average of the energy in the frequency range  $(\omega, \omega + \Delta\omega)$  in the small segment  $(0, a)$  of the string is just the fraction  $(a/l)$  of the (constant) total amount of energy in this frequency range in the entire string.

---

<sup>59</sup>A bar over any quantity denotes the time average of that quantity. The argument that follows, leading to Eqs. (10.14) and (10.17) can also be made in terms of averages over the phases  $\varphi_k$  in the Fourier coefficients in Eq. (10.7).



From Eq. (10.16) it follows that the ( $j \neq k$ ) terms in Eq. (10.12) give the instantaneous deviation  $\Delta E_{(a,\omega)}(t)$  of the energy in this frequency range in the segment  $(0, a)$  of the string from its mean (time average) value:

$$\Delta E_{(a,\omega)}(t) \equiv E_{(a,\omega)}(t) - \overline{E_{(a,\omega)}}(t) = E_{(a,\omega)}^{(j \neq k)}(t). \quad (10.17)$$

We now integrate the ( $j \neq k$ ) terms in Eq. (10.12) to find  $\Delta E_{(a,\omega)}$ . From now on, we suppress the explicit display of the time dependence of  $\Delta E_{(a,\omega)}$ ,  $q_j$  and  $\dot{q}_j$ .

$$\begin{aligned} \Delta E_{(a,\omega)} &= \frac{1}{4} \int_0^a dx \sum_{j \neq k} (\dot{q}_j \dot{q}_k [\cos((\omega_j - \omega_k)x) - \cos((\omega_j + \omega_k)x)] \\ &\quad + \omega_j \omega_k q_j q_k [\cos((\omega_j - \omega_k)x) + \cos((\omega_j + \omega_k)x)]) \\ &= \frac{1}{4} \sum_{j \neq k} \left( \dot{q}_j \dot{q}_k \left[ \frac{\sin((\omega_j - \omega_k)a)}{\omega_j - \omega_k} - \frac{\sin((\omega_j + \omega_k)a)}{\omega_j + \omega_k} \right] \right. \\ &\quad \left. + \omega_j \omega_k q_j q_k \left[ \frac{\sin((\omega_j - \omega_k)a)}{\omega_j - \omega_k} + \frac{\sin((\omega_j + \omega_k)a)}{\omega_j + \omega_k} \right] \right). \end{aligned} \quad (10.18)$$

Defining the expressions within square brackets as (cf. Ch. 4, Eq. (45'))

$$\begin{aligned} K_{jk} &\equiv \frac{\sin((\omega_j - \omega_k)a)}{\omega_j - \omega_k} - \frac{\sin((\omega_j + \omega_k)a)}{\omega_j + \omega_k}, \\ K'_{jk} &\equiv \frac{\sin((\omega_j - \omega_k)a)}{\omega_j - \omega_k} + \frac{\sin((\omega_j + \omega_k)a)}{\omega_j + \omega_k}, \end{aligned} \quad (10.19)$$

we can write this as (cf. Ch. 4, Eq. (45)):

$$\Delta E_{(a,\omega)} = \frac{1}{4} \sum_{j \neq k} (\dot{q}_j \dot{q}_k K_{jk} + \omega_j \omega_k q_j q_k K'_{jk}). \quad (10.20)$$

Note that both  $K_{jk}$  and  $K'_{jk}$  are symmetric:  $K_{jk} = K_{kj}$  and  $K'_{jk} = K'_{kj}$ . We now compute the mean square fluctuation of the energy in the segment  $(0, a)$  in the frequency range  $(\omega, \omega + \Delta\omega)$ . Denoting the two parts of the sum in Eq. (10.20) as  $\Delta E_{1(a,\omega)}$  and  $\Delta E_{2(a,\omega)}$ , respectively, we find (Ch. 4, Eq. (46)):

$$\overline{\Delta E_{(a,\omega)}^2} = \overline{\Delta E_{1(a,\omega)}^2} + \overline{\Delta E_{2(a,\omega)}^2} + \overline{\Delta E_{1(a,\omega)} \Delta E_{2(a,\omega)}} + \overline{\Delta E_{2(a,\omega)} \Delta E_{1(a,\omega)}}. \quad (10.21)$$

Classically, the last two terms are obviously equal to one another. In quantum mechanics we have to be more careful. So it is with malice of forethought that we wrote these last two terms separately. The first two terms are given by (Ch. 4, Eq. (46'))

$$\begin{aligned} \overline{\Delta E_{1(a,\omega)}^2} + \overline{\Delta E_{2(a,\omega)}^2} &= \frac{1}{16} \sum_{j \neq k} \sum_{j' \neq k'} (\overline{\dot{q}_j \dot{q}_k \dot{q}_{j'} \dot{q}_{k'}} K_{jk} K_{j'k'} \\ &\quad + \overline{q_j q_k q_{j'} q_{k'}} \omega_j \omega_k \omega_{j'} \omega_{k'} K'_{jk} K'_{j'k'}); \end{aligned} \quad (10.22)$$

the last two by (Ch. 4, Eq. (46''))

$$\overline{\Delta E_{1(a,\omega)} \Delta E_{2(a,\omega)}} + \overline{\Delta E_{2(a,\omega)} \Delta E_{1(a,\omega)}} = \frac{1}{16} \sum_{j \neq k} \sum_{j' \neq k'} \left( \overline{\dot{q}_j \dot{q}_k q_{j'} q_{k'} \omega_j \omega_k K_{jk} K'_{j'k'}} + \overline{q_j q_k \dot{q}_{j'} \dot{q}_{k'} \omega_j \omega_k K'_{jk} K_{j'k'}} \right). \quad (10.23)$$

Since  $q_k(t) = a_k \cos(\omega_k t + \varphi_k)$  and  $\omega_k = k(\pi/l)$  (see Eqs. (10.6) and (10.7)), it would seem that the time averages of the products of four  $q$ 's or four  $\dot{q}$ 's in Eq. (10.22) vanish unless  $(j = j', k = k')$  or  $(j = k', k = j')$ . This is not strictly true. Writing  $\cos \omega_k t = \frac{1}{2}(e^{i\omega_k t} + e^{-i\omega_k t})$ , we see that there will in principle be non-vanishing contributions whenever  $\pm \omega_j \pm \omega_k \pm \omega_{j'} \pm \omega_{k'} = 0$ .<sup>60</sup> In the real physical situation, however, the string will not be *exactly* fixed at  $x = 0$  and  $x = l$ , which means that the  $\omega$ 's will not *exactly* be integral number times  $(\pi/l)$ . This removes accidental degeneracies of the form  $\pm j \pm k \pm j' \pm k' = 0$  and leaves only the index combinations  $(j = j', k = k')$  and  $(j = k', k = j')$ . These both give the same contribution. Hence (Ch. 4, Eq. (47)):

$$\overline{\Delta E_{1(a,\omega)}^2} + \overline{\Delta E_{2(a,\omega)}^2} = \frac{1}{8} \sum_{j \neq k} \left( \overline{\dot{q}_j^2 \dot{q}_k^2 K_{jk}^2} + \overline{q_j^2 q_k^2 \omega_j^2 \omega_k^2 K_{jk}'^2} \right), \quad (10.24)$$

where we used that, for  $j \neq k$ , averages of products such as  $\overline{\dot{q}_j^2 \dot{q}_k^2}$  are products of the averages  $\overline{\dot{q}_j^2}$  and  $\overline{\dot{q}_k^2}$ . The time averages in Eq. (10.23), with two  $q$ 's and two  $\dot{q}$ 's rather than four  $q$ 's or four  $\dot{q}$ 's, vanish even if  $(j = j', k = k')$  or  $(j = k', k = j')$ . These index combinations produce time averages of expressions of the form  $\sin(\omega_j t + \varphi_j) \cos(\omega_k t + \varphi_k)$  and these vanish. So, in the classical theory, Eq. (10.24) gives the total mean square fluctuation.

To evaluate the mean square averages of the  $q$ 's and  $\dot{q}$ 's in Eq. (10.24), we use the virial theorem, which says that the time average of the kinetic energy of any one of the oscillators in Eq. (10.11) is equal to the time average of its potential energy:

$$\frac{l}{4} \overline{\dot{q}_j^2(t)} = \frac{l}{4} \omega_j^2 \overline{q_j^2(t)} = \frac{1}{2} H_j. \quad (10.25)$$

It follows that

$$\overline{\Delta E_{(a,\omega)}^2} = \frac{1}{2l^2} \sum_{j \neq k} H_j H_k (K_{jk}^2 + K_{jk}'^2). \quad (10.26)$$

We now assume that the energies  $H_j$  of the oscillators of characteristic frequency  $\omega_j$  vary *smoothly* with  $j$ .<sup>61</sup> This assumption, which is not made explicit in the *Dreimännerarbeit*, does not hold for arbitrary distributions of the total energy over the various frequencies,

<sup>60</sup>This problem does not arise if we consider phase averages instead of time averages. Since the phases  $\varphi_j, \varphi_k, \varphi_{j'},$  and  $\varphi_{k'}$  in the  $q$ 's and  $\dot{q}$ 's are statistically independent, the only contributions to Eqs. (10.22) and (10.23) with time averages replaced by phase averages come from terms in the quadruple sum over  $(j \neq k, j' \neq k')$  with either  $(j = j', k = k')$  or  $(j = k', k = j')$ .

<sup>61</sup>What we mean by 'smooth' here is that, if the integers  $j$  are replaced by real numbers  $x$  in the expression for  $H_j$ , the result of integrating the function  $H(x)$  over some interval of the real numbers is negligibly different from the result of taking the discrete sum of terms  $H_j$  over the corresponding range of integers.

but it does hold for many of them. As long as  $H_j$  varies smoothly with  $j$ , we can replace the double sum over  $j$  and  $k$  by a double integral over the continuous variables  $\omega$  and  $\omega'$ . Since  $\omega_j = (\pi/l)j$  (see Eq. (10.6)), a sum over  $j$  turns into  $(l/\pi)$  times an integral over  $\omega$ . Next, we introduce the continuous counterparts  $K_{\omega\omega'}$  and  $K'_{\omega\omega'}$  of  $K_{jk}$  and  $K'_{jk}$ . They are obtained by changing  $\omega_j$  and  $\omega_k$  in Eq. (10.19) into  $\omega$  and  $\omega'$ . When we integrate over the square of  $K_{\omega\omega'}$ , the contribution coming from the square of second term, which has  $\omega + \omega'$  in the denominator, is negligibly small compared to the contribution coming from the square of the first term, which has  $\omega - \omega'$  in the denominator (the integral over the product of the first and the second term vanishes). The same is true for integrals over the square of  $K'_{\omega\omega'}$ .<sup>62</sup> In such integrals  $K_{\omega\omega'}^2$  and  $K'_{\omega\omega'}^2$  can thus be replaced by the squares of their (identical) first terms. Moreover, if  $a$  is very large compared to the wavelengths associated with the frequencies in the narrow range  $(\omega, \omega + \Delta\omega)$ , we can set (cf. Ch. 4, Eq. (48)):

$$\int d\omega' f(\omega') \frac{\sin^2((\omega - \omega')a)}{(\omega - \omega')^2} = \int d\omega' f(\omega') \pi a \delta(\omega - \omega') = \pi a f(\omega), \quad (10.27)$$

where  $\delta(x)$  is the Dirac delta function and  $f(x)$  is an arbitrary function. When we make all these substitutions, Eq. (10.26) turns into:

$$\overline{\Delta E_{(a,\omega)}^2} = \frac{1}{2l^2} \int d\omega \int d\omega' \left(\frac{l}{\pi}\right)^2 2\pi a \delta(\omega - \omega') H_\omega H_{\omega'} = \frac{a}{\pi} \int d\omega H_\omega^2, \quad (10.28)$$

where the integrals are over the interval  $(\omega, \omega + \Delta\omega)$ .<sup>63</sup> Instead of integrating we can multiply the integrand by  $\Delta\omega = 2\pi\Delta\nu$ . If, in addition, we replace functions of  $\omega$  by functions of  $\nu$ , we can write Eq. (10.28) as:

$$\overline{\Delta E_{(a,\nu)}^2} = 2a\Delta\nu H_\nu^2. \quad (10.29)$$

Finally, we replace  $H_\nu$  by the average energy in the frequency range  $(\nu, \nu + \Delta\nu)$  in the segment  $(0, a)$  of the string, using the relation

$$\overline{E_{(a,\nu)}} = N_\nu \left(\frac{a}{l} H_\nu\right), \quad (10.30)$$

where  $N_\nu$  is the number of modes in the interval  $(\nu, \nu + \Delta\nu)$ . Eq. (10.6) tells us that  $\pi N_\nu/l = 2\pi\Delta\nu$ , so

$$N_\nu = 2l\Delta\nu. \quad (10.31)$$

It follows that

$$H_\nu = \frac{\overline{E_{(a,\nu)}}}{2a\Delta\nu}. \quad (10.32)$$

---

<sup>62</sup>It can be shown that neglecting the terms with  $(\omega_j + \omega_k)$  in the denominator in these integrals causes a relative error of order  $\frac{\Delta\omega}{\omega} \frac{1}{a\omega}$ , a product of two factors much smaller than 1.

<sup>63</sup>The corresponding integrals in Eqs. (47'), (49), and (50) are written as integrals from 0 to  $\infty$ , just as the sums in Eqs. (43), (45), (46'), (46''), and (47). After Eq. (49), equivalent to our Eq. (10.28), and Eq. (50) for what in our notation would be  $\overline{E_a}$ , the authors write: "In order to obtain [the thermodynamical mean square energy fluctuation and the mean energy] we have merely to *extract those parts referring to*  $d\nu = d\omega/2\pi$ " (p. 383, our emphasis). This is another clear indication that the authors intended to compute the mean square energy fluctuation in a narrow frequency range.

Inserting this into Eq. (10.29), we arrive at

$$\overline{\Delta E_{(a,\nu)}^2} = \frac{\overline{E_{(a,\nu)}}^2}{2a\Delta\nu} \quad (10.33)$$

for the mean square energy fluctuation in the small segment  $(0, a)$  of the string in the narrow frequency range  $(\nu, \nu + \Delta\nu)$ . This is the analogue of the formula for the mean square energy fluctuation in a narrow frequency range in a small part of a larger volume containing black-body radiation. Eq. (10.33) shows that the mean square fluctuation in the energy is proportional to the mean energy squared.

Eq. (10.33) holds for any state of the string in which there is a smooth distribution of the total energy over the various modes. However, Eq. (10.33) is *not* the formula for the *thermal* mean square energy fluctuation, the quantity that should be compared to Einstein's fluctuation formula of 1909. A clear indication of this is that the temperature  $T$  does not appear anywhere in its derivation. What we need is not a formula for  $\overline{\Delta E_{(a,\nu)}^2}$  in an individual state but a formula for the average  $\langle \overline{\Delta E_{(a,\nu)}^2} \rangle$  in a thermal ensemble of states. Without this extra step, the derivation is incomplete. Neither in the classical nor in the quantum-mechanical version of the calculation, did the authors of the *Dreimännerarbeit* take this extra step.<sup>64</sup> In their defense, we note that when Lorentz (1916) derived his formula for the mean square fluctuation of the energy in a small subvolume of a box with classical electromagnetic radiation, he derived only the analogue of Eq. (10.33) for that system and likewise did not calculate the average of this quantity in a thermal ensemble of states.

Unlike the authors of the *Dreimännerarbeit*, we shall calculate the thermal average of the mean square energy fluctuation formulae they derived, both for the classical formula (10.33) and, at the end of sec. 10.4.2, for the quantum formula (10.59). Classically, a state of the string is fully specified by the amplitudes  $a_k$  and phases  $\varphi_k$  of the infinite number of modes of the string. The thermal average of any observable  $O(a_1, a_2, \dots, \varphi_1, \varphi_2, \dots)$  of the system, which will be some function of these amplitudes and phases, is given by the average over a canonical ensemble of such states:<sup>65</sup>

$$\langle O(a_1, a_2, \dots, \varphi_1, \varphi_2, \dots) \rangle = \frac{\sum_{\{a_1, a_2, \dots, \varphi_1, \varphi_2, \dots\}} O(\dots) e^{-\beta E_{\{a_1, a_2, \dots, \varphi_1, \varphi_2, \dots\}}}}{\sum_{\{a_1, a_2, \dots, \varphi_1, \varphi_2, \dots\}} e^{-\beta E_{\{a_1, a_2, \dots, \varphi_1, \varphi_2, \dots\}}}}. \quad (10.34)$$

The underlying physical picture is that we imagine the string to be coupled to an infinite heat bath at temperature  $T$ , with Boltzmann factor  $\beta \equiv 1/kT$ . We compute the ensemble average of the expression for  $\overline{\Delta E_{(a,\omega)}^2}$  in Eq. (10.26). The only part that we need to be careful about is the product  $H_j H_k$ . So we set  $O$  in Eq. (10.34) equal to:

$$O(a_1, a_2, \dots, \varphi_1, \varphi_2, \dots) = H_j(a_j, \varphi_j) H_k(a_k, \varphi_k). \quad (10.35)$$

<sup>64</sup>This omission was also noted by Wightman (1996, p. 150).

<sup>65</sup>Given that the amplitudes and the phases are continuous quantities, the sums in this equation are symbolic representations of integrals with a measure determined by the transformation from  $\{q_i, p_i\}$  to  $\{a_i, \varphi_i\}$ .

The energy of the string in a given state is just the sum of the Hamiltonians for all the different modes in that state:

$$E_{\{a_1, a_2, \dots, \varphi_1, \varphi_2, \dots\}} = \sum_{i=1}^{\infty} H_i(a_i, \varphi_i). \quad (10.36)$$

It follows that the denominator in Eq. (10.34) can be rewritten as:

$$\sum_{\{a_1, a_2, \dots, \varphi_1, \varphi_2, \dots\}} e^{-\beta \sum_{i=1}^{\infty} H_i(a_i, \varphi_i)} = \prod_{i=1}^{\infty} \left( \sum_{\{a_i, \varphi_i\}} e^{-\beta H_i(a_i, \varphi_i)} \right). \quad (10.37)$$

For all but the  $j^{\text{th}}$  and the  $k^{\text{th}}$  mode, the  $i^{\text{th}}$  factor in the denominator of Eq. (10.34) with  $O = H_j H_k$  cancels against an identical factor in the numerator. Eq. (10.34) thus reduces to the product of two factors of the exact same form, one for the  $j^{\text{th}}$  and one for the  $k^{\text{th}}$  mode. The  $j^{\text{th}}$  mode gives:

$$\frac{\sum_{\{a_j, \varphi_j\}} H_j(a_j, \varphi_j) e^{-\beta H_j(a_j, \varphi_j)}}{\sum_{\{a_j, \varphi_j\}} e^{-\beta H_j(a_j, \varphi_j)}}. \quad (10.38)$$

This is just the ensemble average  $\langle H_j \rangle$  of the  $j^{\text{th}}$  mode. The same is true for the  $k^{\text{th}}$  mode. The equipartition theorem tells us that the average energy of a one-dimensional simple harmonic oscillator at temperature  $T$  is equal to  $kT$ . The modes of the string thus satisfy the analogue of the classical Rayleigh-Jeans law for black-body radiation. Using that  $\langle H_j H_k \rangle = \langle H_j \rangle \langle H_k \rangle$ , we see that the ensemble average of Eq. (10.26) is given by:

$$\overline{\langle \Delta E_{(a, \omega)}^2 \rangle} = \frac{1}{2l^2} \sum_{j \neq k} \langle H_j \rangle \langle H_k \rangle (K_{jk}^2 + K_{jk}'^2). \quad (10.39)$$

Repeating the steps that got us from Eq. (10.26) to Eq. (10.33), we arrive at:

$$\overline{\langle \Delta E_{(a, \nu)}^2 \rangle} = \frac{\langle E_{(a, \nu)} \rangle^2}{2a \Delta \nu}. \quad (10.40)$$

This is the classical formula for the *thermal* mean square fluctuation of the energy in a narrow frequency range in a small segment of the string. Note that in this case the assumption we need to make to replace sums by integrals is that  $\langle H_i \rangle$  varies smoothly with  $i$ , which will certainly be true. In fact, it is a constant:  $\langle H_i \rangle = kT$ . At first sight, it may be surprising that Eq. (10.40) for the thermal average of the mean square energy fluctuation has the same form as Eq. (10.33) for the mean square energy average in an individual state. The reason for this can be gleaned from Eq. (10.26). The entire contribution to the mean square energy fluctuation comes from off-diagonal (i.e.,  $j \neq k$ ) terms involving the product of two distinct, and therefore thermally uncorrelated, modes. This is true for the set of uncoupled oscillators that replaces the string. It is not true for arbitrary systems.

### 10.4.2 Quantum-Mechanical Calculation

In the *Dreimännerarbeit* (pp. 383–384), the classical calculation covered in sec. 10.4.1 is translated into a quantum-mechanical one with the help of Heisenberg's *Umdeutung* procedure. The  $q$ 's and the  $\dot{q}$ 's thus become matrices that do not always commute. The zero-point energy of the harmonic oscillator is a direct consequence of this feature. Another consequence is that the terms in Eq. (10.23), which vanished in the classical case, do contribute to the mean square energy fluctuation in the quantum case. Both this contribution and the zero-point energy of the modes of the string, it turns out, are essential for correctly reproducing the analogue of the particle term in Einstein's fluctuation formula in the simple model used in the *Dreimännerarbeit*.

As we mentioned in the introduction, the key point of Heisenberg's *Umdeutung* paper is that the new quantities representing position and momentum in the new theory still satisfy the classical equations of motion. So the solution for the harmonic oscillator is just the solution of the classical equation of motion for the harmonic oscillator,  $\ddot{q}_k(t) = -\omega_k^2 q_k(t)$ , but now reinterpreted as an equation for matrices. This solution is given by (Baym, 1969, p. 139, Eq. (530)):<sup>66</sup>

$$q_k(t) = q_k(0) \cos \omega_k t + \frac{2p_k(0)}{l\omega_k} \sin \omega_k t. \quad (10.41)$$

Differentiating this equation, we find:

$$\dot{q}_k(t) = \frac{2p_k(0)}{l} \cos \omega_k t - \omega_k q_k(0) \sin \omega_k t. \quad (10.42)$$

In these equations,  $q_k(t)$ ,  $\dot{q}_k(t)$ ,  $q_k(0)$ , and  $p_k(0)$  are all matrices, satisfying the canonical equal-time commutation relations  $[q_j(t), q_k(t)] = 0$ ,  $[p_j(t), p_k(t)] = 0$ , and  $[q_j(t), p_k(t)] = i\hbar\delta_{jk}$ .

An energy eigenstate of the system is given by specifying the values of the infinite set  $\{n_k\}$  of excitation levels of all the modes of the string. The total energy  $E$  of the system in the state  $\{n_k\}$  is the expectation value of the Hamilton operator  $H$  for the whole system in that state. This is the diagonal matrix element  $H(\{n_k\}, \{n_k\})$  (which in modern notation would be  $\langle n_k | H | n_k \rangle$ ):

$$H(\{n_k\}, \{n_k\}) = \sum_{k=1}^{\infty} \left( n_k + \frac{1}{2} \right) \hbar\omega_k. \quad (10.43)$$

The zero-point energy in Eq. (10.43) is clearly infinite. However, as long as we continue to restrict ourselves to a narrow frequency range, the contribution to the zero-point energy will be perfectly finite.

---

<sup>66</sup>Setting  $q_k(0) = a_k \cos \varphi_k$  and  $p_k(0) = -(l\omega_k a_k/2) \sin \varphi_k$  in Eq. (10.41), and interpreting  $q_k(t)$ ,  $\dot{q}_k(t)$ ,  $q_k(0)$ , and  $p_k(0)$  as ordinary numbers, we recover Eq. (10.7):

$$q_k(t) = a_k (\cos \varphi_k \cos \omega_k t - \sin \varphi_k \sin \omega_k t) = a_k \cos(\omega_k t + \varphi_k).$$

In the quantum case, we no longer have the freedom to choose arbitrary phases  $\varphi_k$  that we had in the classical case. Accordingly, we can no longer average over such phases. In the *Dreimännerarbeit* phase averages are simply *defined* as the diagonal part of the quantum-theoretical matrix for the relevant quantity in a basis of energy eigenstates (p. 383).

To find such quantities as the mean energy and the mean square energy fluctuation in a small part of the string and in a narrow frequency range, we first retrace our steps in the classical calculation given above, keeping in mind that  $q$ 's,  $p$ 's, and  $\dot{q}$ 's are no longer numbers but—in modern terminology—operators. We then evaluate the expectation values of the resulting operators in an energy eigenstate of the full system, specified by the excitation levels  $\{n_k\}$ . As in Eq. (10.43), these expectation values are the diagonal matrix elements of the operators in a basis of energy eigenstates. In the *Dreimännerarbeit* the argument is formulated entirely in terms of such matrix elements, but it becomes more transparent if we phrase it in terms of operators and their expectation values. In Ch. 3 of the *Dreimännerarbeit*, on “the connection with the theory of eigenvalues of Hermitian forms,” the authors get close to the notion of operators acting on a state space but they do not use it in the more physical sections of the paper. They clearly recognized, however, that the matrix elements they computed are for states specified by excitation levels of the infinite set of oscillators. The final step, which is not in the *Dreimännerarbeit*, is to compute the average of the quantum expectation value of the relevant operator in a canonical ensemble of energy eigenstates.

Most of the intermediate results in the classical calculation can be taken over unchanged with the understanding that we are now dealing with operators rather than numbers. Replacing the  $q$ 's and  $\dot{q}$ 's (or, equivalently, the  $p$ 's) in Eq. (10.12) for  $E_{(a,\omega)}$  by the corresponding operators and renaming the quantity  $H_{(a,\omega)}$ , we find the Hamilton operator for the small segment  $(0, a)$  of the string in the narrow angular frequency range  $(\omega, \omega + \Delta\omega)$ . This is a perfectly good Hermitian operator, which corresponds, at least in principle, to an observable quantity. We want to emphasize that this is true despite the restriction to a narrow frequency range.

Our first goal is to find the operator  $\overline{\Delta H_{(a,\omega)}^2}$  for the mean square fluctuation of  $H_{(a,\omega)}$ . Eqs. (10.16) and (10.17) for the  $(j = k)$  terms and the  $(j \neq k)$  terms in  $E_{(a,\omega)}$ , respectively, remain valid for the  $(j = k)$  terms and the  $(j \neq k)$  terms of  $H_{(a,\omega)}$ . The  $(j = k)$  terms give the operator for the time average of the energy in the segment  $(0, a)$  in the frequency range  $(\omega, \omega + \Delta\omega)$ :

$$H_{(a,\omega)}^{(j=k)} = \overline{H_{(a,\omega)}}. \quad (10.44)$$

The  $(j \neq k)$  terms give the operator for the instantaneous energy fluctuation in this segment and in this frequency range:

$$H_{(a,\omega)}^{(j \neq k)} = \Delta H_{(a,\omega)} = H_{(a,\omega)} - \overline{H_{(a,\omega)}}. \quad (10.45)$$

This quantity is still given by Eq. (10.20) as long as the  $q$ 's and  $\dot{q}$ 's are read as operators rather than numbers. As before, we split it into two parts,  $\Delta H_{(a,\omega)} = \Delta H_{1(a,\omega)} + \Delta H_{2(a,\omega)}$ . Thus, as in Eq. (10.21), the operator  $\overline{\Delta H_{(a,\omega)}^2}$  for the mean square fluctuation of the energy in the small segment  $(0, a)$  in the frequency range  $(\omega, \omega + \Delta\omega)$  is given by four terms. The first two terms are still given by Eq. (10.26),<sup>67</sup> the last two by Eq. (10.23) (with  $E$  replaced by  $H$ ). The latter vanished in the classical case but not in the quantum

---

<sup>67</sup>As the authors explicitly note, the virial theorem, which was used to get from Eq. (10.24) to Eq. (10.26), remains valid in matrix mechanics (pp. 343 and 383).

case (p. 384).<sup>68</sup> These terms now give identical contributions for the index combinations  $(j = j', k = k')$  and  $(j = k', k = j')$  with  $j \neq k$  and  $j' \neq k'$ . The quadruple sum in Eq. (10.23) reduces to the double sum:

$$\begin{aligned} & \overline{\Delta H_{1(a,\omega)} \Delta H_{2(a,\omega)}} + \overline{\Delta H_{2(a,\omega)} \Delta H_{1(a,\omega)}} \\ &= \frac{1}{8} \sum_{j \neq k} (\overline{\dot{q}_j q_j \dot{q}_k q_k} + \overline{q_j \dot{q}_j q_k \dot{q}_k}) \omega_j \omega_k K_{jk} K'_{jk}, \end{aligned} \quad (10.46)$$

where we used that  $q_j$  commutes with  $\dot{q}_k$  as long as  $j \neq k$ . The two terms in Eq. (10.46), it turns out, give identical contributions. We focus on the first. We compute the time average  $\overline{\dot{q}_j q_j}$ . Using Eqs. (10.41) and (10.42), we find that

$$\overline{\dot{q}_j q_j} = \overline{\left( \frac{2p_j(0)}{l} \cos \omega_j t - \omega_j q_j(0) \sin \omega_j t \right) \left( q_j(0) \cos \omega_j t + \frac{2p_j(0)}{l\omega_j} \sin \omega_j t \right)},$$

which reduces to

$$\overline{\dot{q}_j q_j} = \frac{1}{l} (p_j(0)q_j(0) - q_j(0)p_j(0)). \quad (10.47)$$

Classically,  $p$  and  $q$  commute, but in quantum theory we have  $[q_j(0), p_j(0)] = i\hbar$ , so that

$$\overline{\dot{q}_j q_j} = -\frac{i\hbar}{l}. \quad (10.48)$$

The time average  $\overline{q_j \dot{q}_j}$  is likewise given by  $i\hbar/l$ . Inserting these results into Eq. (10.46), we find

$$\overline{\Delta H_{1(a,\omega)} \Delta H_{2(a,\omega)}} + \overline{\Delta H_{2(a,\omega)} \Delta H_{1(a,\omega)}} = -\frac{\hbar^2}{4l^2} \sum_{j \neq k} \omega_j \omega_k K_{jk} K'_{jk}. \quad (10.49)$$

When we add the contributions to  $\overline{\Delta H_{(a,\omega)}^2}$  coming from Eq. (10.49) to those coming from Eq. (10.26), we find

$$\overline{\Delta H_{(a,\omega)}^2} = \frac{1}{l^2} \sum_{j \neq k} \left( H_j H_k \frac{1}{2} (K_{jk}^2 + K'_{jk}{}^2) - \frac{\hbar^2}{4} \omega_j \omega_k K_{jk} K'_{jk} \right). \quad (10.50)$$

---

<sup>68</sup>This is the step that Born and Fuchs (1939a, p. 263) complained involved “quite incomprehensible reasoning” (cf. note 26). They wrote: “The error in the paper of Born, Heisenberg, and Jordan is in the evaluation of the terms  $\Delta_1 \Delta_2 + \Delta_2 \Delta_1$  (see formula (46'') [p. 382; our Eq. (10.23)]). On [p. 382] it is correctly stated that in the classical calculation the mean value of this quantity over all phases vanishes. This is also true in the quantum mechanical calculation as is apparent from formula (46''). [On the bottom half of p. 384], however,  $\Delta_1 \Delta_2 + \Delta_2 \Delta_1$  reappears again with a non-vanishing value [cf. our Eq. (10.49)] and it is shown that it gives rise to an additional term by means of quite incomprehensible reasoning. It is just this term which transforms the correct formula (2.1) [the mean square energy fluctuation for classical waves; cf. our Eq. (10.33)] into the thermodynamical formula (1.6) [Einstein's fluctuation formula]. But from the standpoint of wave theory this formula (1.6) is certainly wrong” (ibid.). As we shall see, there is nothing wrong with this step in the argument in the *Dreimännerarbeit*. We suspect that what tripped up Born in 1939 was the distinction between phase averages and time averages in the *Dreimännerarbeit*.



Replacing both  $\frac{1}{2} (K_{jk}^2 + K'_{jk}{}^2)$  and  $K_{jk}K'_{jk}$  by  $\sin^2((\omega_j - \omega_k)a)/(\omega_j - \omega_k)^2$  (cf. the paragraph before Eq. (10.27)), we can rewrite Eq. (10.50) as

$$\overline{\Delta H_{(a,\omega)}^2} = \frac{1}{l^2} \sum_{j \neq k} \left( H_j H_k - \frac{\hbar^2}{4} \omega_j \omega_k \right) \frac{\sin^2((\omega_j - \omega_k)a)}{(\omega_j - \omega_k)^2}. \quad (10.51)$$

The next step—and the final step in the *Dreimännerarbeit*—is to evaluate the expectation value of the operator  $\Delta H_{(a,\omega)}^2$  in the state  $\{n_i\}$ . This is the diagonal matrix element,  $\overline{\Delta H_{(a,\omega)}^2}(\{n_i\}, \{n_i\})$ .<sup>69</sup> Using that

$$H_j(\{n_i\}, \{n_i\}) = \left( n_j + \frac{1}{2} \right) \hbar \omega_j, \quad (10.52)$$

we find that

$$\begin{aligned} \overline{\Delta E_{(a,\omega)}^2} &\equiv \overline{\Delta H_{(a,\omega)}^2}(\{n_i\}, \{n_i\}) \\ &= \frac{1}{l^2} \sum_{j \neq k} \left( \left( n_j + \frac{1}{2} \right) \left( n_k + \frac{1}{2} \right) - \frac{1}{4} \right) \hbar^2 \omega_j \omega_k \frac{\sin^2((\omega_j - \omega_k)a)}{(\omega_j - \omega_k)^2} \\ &= \frac{1}{l^2} \sum_{j \neq k} \left( n_j n_k + \frac{1}{2} (n_j + n_k) \right) \hbar^2 \omega_j \omega_k \frac{\sin^2((\omega_j - \omega_k)a)}{(\omega_j - \omega_k)^2}. \end{aligned} \quad (10.53)$$

We thus see that the contribution to the mean square fluctuation coming from the second term in Eq. (10.50), which comes from the non-commutativity of  $q$  and  $p$ , cancels the square of the zero-point energy in the contribution coming from the first term.

Eq. (10.53) also illustrates the problem that Heisenberg (1931) drew attention to a few years later (see sec. 10.3.2). If we let  $j$  and  $k$  run from 1 to  $\infty$  instead of restricting them to some finite interval, the double sum in Eq. (10.53) diverges. The problem comes from the terms with  $(n_j + n_k)$ ; the contribution coming from the terms with  $n_j n_k$  will still be perfectly finite, at least after we have made the transition from individual states to a thermal ensemble of states. In that case, the excitation level  $n_i$  drops off exponentially with  $i$  (see Eq. (10.60)), so the double sum over the terms with  $n_j n_k$  will quickly converge. This is not the case for the terms with just  $n_j$  or just  $n_k$ . For a fixed value of  $j$ , for instance,<sup>70</sup> the double sum over the term with  $n_j$  in Eq. (10.53) will reduce to the single sum:

$$\frac{n_j \hbar^2 \omega_j}{2l^2} \sum_{k=1 (k \neq j)}^{\infty} \omega_k \frac{\sin^2((\omega_j - \omega_k)a)}{(\omega_j - \omega_k)^2}. \quad (10.54)$$

<sup>69</sup>We remind the reader that the authors of the *Dreimännerarbeit* do not explicitly distinguish between operators and their expectation values. This is a source of possible confusion at this point. The authors write: “we denote those parts of  $\overline{\Delta^2}$  [rendered in bold] which belong to a given frequency  $\nu$  as  $\overline{\Delta^2}$  [not rendered in bold]” (p. 384). Without any further information, one can read this either as a restriction (in our notation) of the operator  $\overline{\Delta H_a^2}$  to the operator  $\overline{\Delta H_{(a,\omega)}^2}$  or as a restriction of the states  $\{n_i\}$  in the matrix element  $\overline{\Delta H_a^2}(\{n_i\}, \{n_i\})$  to states in which only modes in the frequency interval  $\omega < i(\pi/l) < \omega + \Delta\omega$  are present (i.e.,  $n_i = 0$  for all frequencies  $i(\pi/l)$  outside that narrow range). Since the latter reading makes no sense (we are interested in states with excitations over the whole frequency spectrum), we assume that the former reading is what the authors had in mind. We are grateful to Jürgen Ehlers for alerting us to this ambiguity.

<sup>70</sup>For fixed values of  $k$ , we run into the same problem.

This sum is logarithmically divergent. Following Heisenberg's suggestion in 1931, we can remedy this divergence if we replace the sharp edge of the segment of the string at  $a$  by a smooth edge. Integration over the segment  $(0, a)$  of the string is equivalent to integration over the whole string if we multiply the integrand by the theta-function  $\vartheta(a-x)$  (defined as:  $\vartheta(\xi) = 0$  for  $\xi < 0$  and  $\vartheta(\xi) = 1$  for  $\xi \geq 0$ ). The Fourier coefficients for this theta-function do not fall off fast enough if  $j$  or  $k$  go to infinity. This is why the factors  $K_{jk}$  and  $K'_{jk}$  in Eq. (10.19) do not fall off fast enough either if  $j$  or  $k$  go to infinity. If we replace the theta-function by a smooth, infinitely differentiable function, the problem disappears, since in that case the Fourier transform will fall off faster than any power of the transform variables  $j$  or  $k$ . We emphasize that as long as the sums in Eq. (10.53) are restricted to a finite frequency interval, the result is finite without any such remedy.

As in the classical calculation (cf. Eqs. (10.26)–(10.29)), we make the transition from sums to integrals. We can do this as long as the excitation levels  $n_j$  vary smoothly with  $j$ . We can then replace the double sum over  $j$  and  $k$  by  $(l/\pi)^2$  times a double integral over  $\omega$  and  $\omega'$  and  $n_j$  and  $n_k$  by  $n_\omega$  and  $n_{\omega'}$ . We can also replace  $\sin^2((\omega - \omega')a)/(\omega - \omega')^2$  by  $\pi a \delta(\omega - \omega')$  (see Eq. (10.27)). Eq. (10.53) then turns into:

$$\begin{aligned} \overline{\Delta E_{(a,\omega)}^2} &= \frac{a}{\pi} \int d\omega \int d\omega' \delta(\omega - \omega') \left( n_\omega n_{\omega'} + \frac{1}{2} (n_\omega + n_{\omega'}) \right) \hbar^2 \omega \omega' \\ &= \frac{a}{\pi} \int d\omega (n_\omega^2 + n_\omega) \hbar^2 \omega^2. \end{aligned} \quad (10.55)$$

Replacing integration over the interval  $(\omega, \omega + \Delta\omega)$  by multiplication by  $\Delta\omega = 2\pi\Delta\nu$  and writing all quantities as functions of  $\nu$  rather than  $\omega$ , we find:

$$\overline{\Delta E_{(a,\nu)}^2} \equiv \overline{\Delta H_{(a,\nu)}^2}(\{n_\nu\}, \{n_\nu\}) = 2a\Delta\nu ((n_\nu h\nu)^2 + (n_\nu h\nu)h\nu). \quad (10.56)$$

We now introduce the excitation energy, the difference between the total energy and the zero-point energy. Jordan and his co-authors call this the “thermal energy” (p. 377, p. 384). Although the intuition behind it is clear (cf. note 73), this terminology is misleading. The term ‘thermal energy’ suggests that the authors consider a thermal ensemble of energy eigenstates, what we would call a mixed state, while in fact they are dealing with individual energy eigenstates, i.e., pure states. We therefore prefer the term ‘excitation energy’. The excitation energy  $E_\nu$  in the narrow frequency range  $(\nu, \nu + \Delta\nu)$  in the entire string in the state  $\{n_\nu\}$  is:

$$E_\nu = N_\nu(n_\nu h\nu) = 2l\Delta\nu(n_\nu h\nu), \quad (10.57)$$

where we used that  $N_\nu = 2l\Delta\nu$  is the number of modes between  $\nu$  and  $\nu + \Delta\nu$  (see Eq. (10.31)). On average there will be a fraction  $a/l$  of this energy in the small segment  $(0, a)$  of the string (p. 384, equation following Eq. (54)):<sup>71</sup>

$$\overline{E_{(a,\nu)}} = \frac{a}{l} E_\nu = 2a\Delta\nu(n_\nu h\nu). \quad (10.58)$$

---

<sup>71</sup>The time average  $\overline{E_{(a,\nu)}}$  of the excitation energy in the narrow frequency range  $(\nu, \nu + \Delta\nu)$  in the small segment  $(0, a)$  of the string in the state  $\{n_\nu\}$  is the expectation value of the operator  $\overline{H_{(a,\nu)}} - \frac{1}{2}h\nu$  in that state.

Substituting  $\overline{E_{(a,\nu)}}/2a\Delta\nu$  for  $n_\nu h\nu$  in Eq. (10.56), we arrive at the final result of this section of the *Dreimännerarbeit* (Ch. 4, Eq. (55)):

$$\overline{\Delta E_{(a,\nu)}^2} = \frac{\overline{E_{(a,\nu)}}^2}{2a\Delta\nu} + \overline{E_{(a,\nu)}}h\nu. \quad (10.59)$$

Like Eq. (10.33) in the classical case, Eq. (10.59) holds for any state with a smooth distribution of energy over frequency. Unlike the classical formula, however, Eq. (10.59) has exactly the same form as Einstein's fluctuation formula of 1909 (see the third line of Eq. (10.3)). The first term has the form of the classical wave term (cf. Eq. (10.33)); the second term has the form of a particle term.

As in the classical case, however, we are not done yet. Eq. (10.59), like Eq. (10.33), is for individual states, whereas what we need is a formula for a thermal ensemble of states. In quantum mechanics, this transition from an individual state (a pure state) to an ensemble of states (a mixed state) is a little trickier than in classical theory. Before we show how this is done, we want to make some comments about the interpretation of Eq. (10.59) to make it clear that this formula does not give the *thermal* mean square energy fluctuation. In modern terms, the formula is for the mean square *quantum uncertainty* or *quantum dispersion* in the energy in a narrow frequency range in a small segment of the string when the whole string is in an energy eigenstate  $\{n_\nu\}$ . The operators  $H$  and  $H_{(a,\nu)}$  do not commute. The system is in an eigenstate of the full Hamiltonian  $H$  but in a superposition of eigenstates of the Hamiltonian  $H_{(a,\nu)}$  of the subsystem. Eq. (10.59) is a measure for the spread in the eigenvalues of the eigenstates of  $H_{(a,\nu)}$  that make up this superposition rather than a measure of the spread in the value of the energy in the subsystem in an thermal ensemble of eigenstates of the system as a whole. It is that latter spread that gives the thermal mean square energy fluctuation.

Proceeding as we did in the classical case (see Eqs. (10.34)–(10.40)), we make the transition from the formula for the mean square quantum uncertainty of the energy of the subsystem in an energy eigenstate of the whole system to the formula for the mean square fluctuation of this quantity in an ensemble of such states. As in the classical case, it turns out that these two formulae have the same form. The reason for this is once again that the entire contribution to the mean square energy fluctuation in Eq. (10.59) comes from off-diagonal (i.e.,  $j \neq k$ ) terms involving the product of two distinct, and therefore thermally uncorrelated, modes, as can clearly be seen, for instance, in Eq. (10.51). The thermal average of the product  $H_j H_k$  is the product of the thermal averages of  $H_j$  and  $H_k$ . This is a special feature of the system of uncoupled harmonic oscillators that we are considering and will not hold in general. In this special case, it turns out, we get from the formula for a single state to the formula for a thermal ensemble of states simply by replacing the excitation levels  $n_i$  in Eq. (10.53) by the thermal excitation levels given by the Planck function.<sup>72</sup>

$$\hat{n}_j \equiv \frac{1}{e^{kT/h\nu_j} - 1}, \quad (10.60)$$

and repeat the steps that took us from Eq. (10.53) to Eq. (10.59).

---

<sup>72</sup>The criticism at this point in the *Dreimännerarbeit* (p. 379) of the statistics that Debye (1910) used to recover the Planck function (see also Jordan to Einstein, October 29, 1925 [AE 13-473]) is retracted in (Jordan, 1928, p. 182, note).

We now show this in detail, taking Eq. (10.51) as our starting point. We imagine the string to be coupled to an infinite external heat bath at temperature  $T$ . The value of some observable in thermal equilibrium is given by the canonical-ensemble expectation value of the diagonal matrix elements of the corresponding operator  $O$  in eigenstates  $\{n_i\}$  of the Hamiltonian for the system as a whole:

$$\langle O(\{n_i\}, \{n_i\}) \rangle = \frac{\sum_{\{n_i\}} O(\{n_i\}, \{n_i\}) e^{-\beta E_{\{n_i\}}}}{\sum_{\{n_i\}} e^{-\beta E_{\{n_i\}}}}, \quad (10.61)$$

where  $E_{\{n_i\}} = \sum_{n_i} (n_i + \frac{1}{2}) \hbar \omega_i$  (see Eq. (10.43)).<sup>73</sup> We calculate the thermal average of the diagonal matrix elements of the operator  $\overline{\Delta H_{(a,\omega)}^2}$  in the state  $\{n_i\}$ :  $\langle \overline{\Delta H_{(a,\omega)}^2}(\{n_i\}, \{n_i\}) \rangle$ . The only non-trivial part of this calculation is to determine the thermal average of the matrix elements  $H_j H_k(\{n_i\}, \{n_i\})$  (with  $j \neq k$ ). These matrix elements are given by (cf. Eq. (10.53)):

$$H_j H_k(\{n_i\}, \{n_i\}) = \left(n_j + \frac{1}{2}\right) \hbar \omega_j \left(n_k + \frac{1}{2}\right) \hbar \omega_k. \quad (10.62)$$

For the thermal average of this expression, we find, using Eq. (10.61):

$$\langle H_j H_k(\{n_i\}, \{n_i\}) \rangle = \frac{\sum_{\{n_i\}} \left(n_j + \frac{1}{2}\right) \hbar \omega_j \left(n_k + \frac{1}{2}\right) \hbar \omega_k e^{-\beta E_{\{n_i\}}}}{\sum_{\{n_i\}} e^{-\beta E_{\{n_i\}}}}. \quad (10.63)$$

The sum over all possible states  $\{n_i\}$  in the denominator can be written as a product of sums over all possible values of the excitation level  $n_i$  for all modes  $i$ :

$$\sum_{\{n_i\}} e^{-\beta E_{\{n_i\}}} = \prod_{i=1}^{\infty} \left( \sum_{n_i=1}^{\infty} e^{-\beta \left(n_i + \frac{1}{2}\right) \hbar \omega_i} \right). \quad (10.64)$$

For all but the  $j^{\text{th}}$  and the  $k^{\text{th}}$  mode the  $i^{\text{th}}$  factor in the denominator cancels against an identical factor in the numerator. Eq. (10.63) thus reduces to a product of two factors of the same form, one for the  $j^{\text{th}}$  mode and one for the  $k^{\text{th}}$  mode. Consider the former:

$$\frac{\sum_{n_j} \left(n_j + \frac{1}{2}\right) \hbar \omega_j e^{-\beta (n_j + \frac{1}{2}) \hbar \omega_j}}{\sum_{n_j} e^{-\beta (n_j + \frac{1}{2}) \hbar \omega_j}} = \frac{1}{2} \hbar \omega_j + \frac{\sum_{n_j} n_j \hbar \omega_j e^{-\beta n_j \hbar \omega_j}}{\sum_{n_j} e^{-\beta n_j \hbar \omega_j}}. \quad (10.65)$$

---

<sup>73</sup>It does not matter for the ensemble average whether or not we include the zero-point energy in  $E_{\{n_i\}}$ , since the contributions from the zero-point energy to numerator and denominator are the same and cancel. This clearly is what Jordan was getting at when he introduced the term 'thermal energy' for what we proposed to call the excitation energy (see the passage from his letter to Einstein of December 15, 1925, quoted in sec. 10.3.7).

The expression in the denominator in the second term on the right-hand side is a geometric series, which we shall call  $Z$ :

$$Z \equiv \sum_{n_j} e^{-\beta n_j \hbar \omega_j} = \frac{1}{1 - e^{-\beta \hbar \omega_j}}. \quad (10.66)$$

The fraction of the two sums in Eq. (10.65) is just minus the derivative of  $\ln Z$  with respect to  $\beta$ . Eq. (10.66) allows us to write this as:

$$-\frac{d}{d\beta} \ln Z = -\frac{1}{Z} \frac{dZ}{d\beta} = -\left(1 - e^{-\beta \hbar \omega_j}\right) \frac{-\hbar \omega_j e^{-\beta \hbar \omega_j}}{(1 - e^{-\beta \hbar \omega_j})^2} = \frac{\hbar \omega_j}{e^{\beta \hbar \omega_j} - 1}, \quad (10.67)$$

which is equal to  $\hat{n}_j \hbar \omega_j$ , where we used Eq. (10.60) for the thermal excitation levels. The right-hand side of Eq. (10.65) thus becomes  $(\hat{n}_j + \frac{1}{2}) \hbar \omega_j$ . Using this result for the  $j^{\text{th}}$  mode and a similar result for  $k^{\text{th}}$  mode, we can write Eq. (10.63) as

$$\begin{aligned} \langle H_j H_k(\{n_i\}, \{n_i\}) \rangle &= \langle H_j(\{n_i\}, \{n_i\}) \rangle \langle H_k(\{n_i\}, \{n_i\}) \rangle \\ &= \left(\hat{n}_j + \frac{1}{2}\right) \hbar \omega_j \left(\hat{n}_k + \frac{1}{2}\right) \hbar \omega_k. \end{aligned} \quad (10.68)$$

Using this result, we calculate the thermal average of the diagonal matrix elements in the state  $\{n_i\}$  of the operator in Eq. (10.51) for the mean square energy fluctuation in a narrow frequency interval in a small segment of the string:

$$\begin{aligned} \overline{\langle \Delta E_{(a,\omega)}^2 \rangle} &\equiv \overline{\langle \Delta H_{(a,\omega)}^2(\{n_i\}, \{n_i\}) \rangle} \\ &= \frac{1}{j^2} \sum_{j \neq k} \left( \hat{n}_j \hat{n}_k + \frac{1}{2} (\hat{n}_j + \hat{n}_k) \right) \hbar^2 \omega_j \omega_k \frac{\sin^2((\omega_j - \omega_k)a)}{(\omega_j - \omega_k)^2}. \end{aligned} \quad (10.69)$$

The right-hand side has exactly the same form as Eq. (10.53), except that the  $n$ 's are replaced by  $\hat{n}$ 's. Eq. (10.60) tells us that  $\hat{n}_j$  and  $\hat{n}_k$  vary smoothly with  $j$  and  $k$ , so we can make the transition from sums to integrals in this case without any further assumptions. Proceeding in the exact same way as we did to get from Eq. (10.53) to Eq. (10.56), we arrive at:

$$\overline{\langle \Delta E_{(a,\nu)}^2 \rangle} = 2a\Delta\nu \left( (\hat{n}_\nu h\nu)^2 + (\hat{n}_\nu h\nu)\nu \right). \quad (10.70)$$

The thermal average of the mean excitation energy in a narrow frequency interval in a small segment of the string is given by (cf. Ch. 4, Eq. (39))

$$\overline{\langle E_{(a,\nu)} \rangle} = \frac{a}{l} (\hat{n}_\nu h\nu) N_\nu = 2a\Delta\nu (\hat{n}_\nu h\nu). \quad (10.71)$$

This is just Eq. (10.58) with  $\hat{n}$  instead of  $n$ . With the help of this expression we can rewrite Eq. (10.70) as:

$$\overline{\langle \Delta E_{(a,\nu)}^2 \rangle} = \frac{\overline{\langle E_{(a,\nu)} \rangle}^2}{2a\Delta\nu} + \overline{\langle E_{(a,\nu)} \rangle} h\nu. \quad (10.72)$$

This formula for the canonical-ensemble average of the mean square fluctuation of the energy in a narrow frequency range in a small segment of the string has exactly the same form as Eq. (10.59) for the mean square quantum uncertainty in the energy of this subsystem in an energy eigenstate of the system as a whole.

Our final result, Eq. (10.72), is the analogue of Einstein's famous 1909 formula for the mean square fluctuation of the energy in a narrow frequency range in a subvolume of a box with black-body radiation. That Eq. (10.72) emerges from the quantum-mechanical treatment of the modes of a string shows that the fluctuation formula, contrary to what Einstein thought, does not call for two separate mechanisms, one involving particles and one involving waves. In matrix mechanics, both terms arise from a unified dynamical framework. In the *Dreimännerarbeit* this unified mechanism is described in terms of quantized waves. If we focus on the occupation levels  $n_i$  rather than on the field  $u(x, t)$ , however, we see that the same mechanism can also be described in terms of particles, quanta of the field, satisfying Bose's statistics.

## **10.5 Assessment of the Validity and the Importance of Jordan's Argument**

The main conclusion we want to draw from our reconstruction of the fluctuation considerations in the *Dreimännerarbeit* is that they support the authors' claim—or rather Jordan's claim—that a straightforward application of the new matrix mechanics to a simple model of black-body radiation, viz. oscillations in a string fixed at both ends, leads to an expression for the mean square energy fluctuation in a narrow frequency range in a small segment of that string that has exactly the same form as the formula Einstein derived from statistical mechanics and Planck's black-body radiation law for the mean square energy fluctuation in a narrow frequency range in a subvolume of a box filled with black-body radiation. We also noted, however, that the authors use a sloppy notation and that the argument they present is incomplete.

At various points, the notation fails to reflect the crucial restriction to a narrow frequency range. We drew attention to a couple of passages in the text that clearly indicate that such a restriction is nonetheless in effect throughout the calculation. Since the entire derivation is for a finite frequency range, there are no problems with infinities (*pace* Ehlers, 2007, pp. 28–29). Another problem is that the authors do not distinguish in their notation between (in modern terms) operators and expectation values of operators in energy eigenstates. Here we have to keep in mind that this distinction had not fully crystalized when the paper was written. The authors had no clear notion yet of operators acting on states. They did not even have the general concept of a state (Duncan and Janssen, 2007, sec. 3).

In the absence of the general state concept, they did not distinguish between pure states and mixed states either. This did trip them up. The formula they derived is for the mean square *quantum uncertainty* in the energy of a subsystem in an energy eigenstate of the system as a whole, which is a *pure state*. What they should have derived to recover Einstein's fluctuation formula is a formula for the *thermal* mean square fluctuation in the energy of the subsystem, i.e., a canonical-ensemble average over energy eigenstates of the whole system, which is a *mixed state*. We showed in detail how to make this transition from quantum uncertainty to thermal fluctuations. Given the preliminary

character of the theory he was working with, Jordan can be forgiven for the omission of this step in the *Dreimännerarbeit*, though he probably should have known better when he presented his result again in later publications. In Jordan's defense, we noted that Lorentz likewise omitted the corresponding step in the classical calculation.

With our admittedly not unimportant emendation, Jordan's result resolves Einstein's conundrum of the wave-particle duality of light, even though the treatment of such phenomena as the photoelectric effect and the Compton effect had to await the work of Dirac (1927), who developed the theory for the interaction between the quantized electromagnetic field and matter. As we saw in sec. 10.3.6, Jordan emphasized his resolution of the wave-particle conundrum in a number of publications. The main reason for the lukewarm reception of this result in the physics community of his day seems to have been that it looked suspicious because of the infinities one already encounters in this simple example of a quantum theory of free fields. This suspicion has lingered, even though, as we saw, Jordan managed to steer clear of infinities by focusing on a narrow frequency range.

The less than enthusiastic reaction of the physicists no doubt partly explains why Jordan's result has not become a staple of the historical literature on the wave-particle duality of light. Another factor responsible for its neglect in this context, as we suggested in sec. 10.3, may have been that Jordan's result was too many things at once. It was the resolution of the conundrum of the wave-particle duality of light but it was also a striking piece of evidence for matrix mechanics and a telltale sign that a quantum theory of fields was needed. Given how strongly Jordan felt about this last use of his result, it is perhaps only fitting that his derivation of Einstein's fluctuation formula has found its place in the historical literature not toward the end of histories of wave-particle duality but at the beginning of histories of quantum field theory. Still, the result only played a relatively minor role in the early stages of quantum mechanics and quantum field theory. By contrast, it is the denouement of the early history of the wave-particle duality of light. Regrettably, it has either been ignored in that context or doubts have been cast upon it. We hope that our paper will help remove those doubts so that Jordan's result can finally be given its rightful place in the heroic tale of Einstein, light quanta, and the wave-particle duality of light.

**Acknowledgments** A preliminary version of this paper was presented at HQ-1, a conference on the history of quantum physics held at the *Max-Planck-Institut für Wissenschaftsgeschichte*, Berlin, July 2–6, 2007. We thank Clayton Gearhart, Don Howard, Joska Illy, Alexei Kojevnikov, Serge Rudaz, Rob Rynasiewicz, John Stachel, Jos Uffink, two anonymous referees, and, especially, Jürgen Ehlers for helpful comments, discussion, and references. We thank Michael Jordan for permission to quote extensively from his father's unpublished correspondence and from the interview with his father for the *Archive for History of Quantum Physics* (AHQP). We likewise thank Jochen Heisenberg for permission to quote from an unpublished letter from his father, which is available in microfilm as part of the AHQP. We also thank the staff at Walter Library at the University of Minnesota, where we consulted a copy of the AHQP. Finally, we thank the Einstein Archive at Hebrew University and Princeton University Press for permission to quote an unpublished postcard from Einstein to Jordan. The research of Anthony Duncan is supported in part by the National Science Foundation under grant PHY-0554660.

## Bibliography

- Bach, A. (1989). Eine Fehlinterpretation mit Folgen: Albert Einstein und der Welle-Teilchen Dualismus. *Archive for History of Exact Sciences* 40: 173–206.
- Balashov, Y., and Vizgin, V. eds. (2002), *Einstein studies in Russia*. Boston: Birkhäuser.
- Baym, G. (1969). *Lectures on quantum mechanics*. Reading, MA: Addison-Wesley.
- Beyler, R. H. (1969). Exporting the quantum revolution: Pascual Jordan's biophysical initiatives. In (Hoffmann *et al.*, 2007, pp. 69–81)
- Bohr, N., Kramers, H. A., and Slater, J. C. (1924a). The quantum theory of radiation *Philosophical Magazine* 47: 785–802. Reprinted in (Van der Waerden, 1968, pp. 159–176).
- Born, M. (1925). *Vorlesungen über Atommechanik*. Berlin: Springer.
- Born, M. (1978). *My life. Recollections of Nobel laureate*. New York: Charles Scribner.
- Born, M., and Fuchs, K. (1939a). On fluctuations in electromagnetic radiation. *Proceedings of the Royal Society of London, Series A, Mathematical and Physical Sciences*. 170: 252–265.
- Born, M., and Fuchs, K. (1939b). On fluctuations in electromagnetic radiation. (A correction.) *Proceedings of the Royal Society of London, Series A, Mathematical and Physical Sciences*. 172: 465–466.
- Born, M., Heisenberg, W., and Jordan, P. (1926). Zur Quantenmechanik II. *Zeitschrift für Physik* 35: 557–615. Page references to the English translation in (Van der Waerden, 1968, pp. 321–385).
- Born, M., and Jordan, P. (1925). Zur Quantenmechanik. *Zeitschrift für Physik* 34: 858–888. Page references are to the English translation of chs. 1–3 in (Van der Waerden, 1968, pp. 277–306). Ch. 4 is omitted in this translation.
- Born, M., and Jordan, P. (1930). *Elementare Quantenmechanik*. Berlin: Springer.
- Bose, S. N. (1924). Plancks Gesetz und Lichtquantenhypothese. *Zeitschrift für Physik* 26: 178–181.
- Bothe, W. (1923). Die räumliche Energieverteilung in der Hohlraumstrahlung. *Zeitschrift für Physik* 20: 145–152.
- Bothe, W. (1924). Über die Wechselwirkung zwischen Strahlung und freien Elektronen. *Zeitschrift für Physik* 23: 214–224.



- Bothe, W. (1927). Zur Statistik der Hohlraumstrahlung. *Zeitschrift für Physik* 41: 345–351
- Camilleri, K. (2006). Heisenberg and the wave-particle duality. *Studies in the History and Philosophy of Modern Physics* 37: 298–315.
- Cini, M. (2003). Field quantization and wave particle duality. *Annals of Physics* 305: 83–95.
- Darrigol, O. (1986). The origin of quantized matter waves. *Historical Studies in the Physical and Biological Sciences* 16: 197–253.
- Debye, P. (1910). Der Wahrscheinlichkeitsbegriff in der Theorie der Strahlung. *Annalen der Physik* 33: 1427–1434.
- Dirac, P.A.M. (1926). On the theory of quantum mechanics. *Proceedings of the Royal Society of London, Series A, Mathematical and Physical Sciences*. 112: 661–677.
- Dirac, P.A.M. (1927). The quantum theory of the emission and absorption of radiation. *Proceedings of the Royal Society of London, Series A, Mathematical and Physical Sciences*. 114: 243–265. Reprinted in (Schwinger, 1958, pp. 1–23)
- Duncan, A., and Janssen, M. (2007). On the verge of *Umdeutung* in Minnesota: Van Vleck and the correspondence principle. 2 Pts. *Archive for History of Exact Sciences* 61: 553–624, 625–671.
- Ehlers, J. (2007). Pascual Jordan's role in the creation of quantum field theory. In (Hoffmann *et al.*, 2007, pp. 23–35).
- Ehrenfest, P. (1925). Energieschwankungen im Strahlungsfeld oder Kristallgitter bei Superposition quantisierter Eigenschwingungen. *Zeitschrift für Physik* 34: 362–373.
- Einstein, A. (1904). Zur allgemeinen molekularen Theorie der Wärme *Annalen der Physik* 14: 354–362. Reprinted in facsimile as Doc. 5 in (Einstein, 1987–2006, Vol. 2).
- Einstein, A. (1905). Über einen die Erzeugung und Verwandlung des Lichtes betreffenden heuristischen Gesichtspunkt. *Annalen der Physik* 17: 132–148. Reprinted in facsimile as Doc. 14 in (Einstein, 1987–2006, Vol. 2).
- Einstein, A. (1909a). Zum gegenwärtigen Stand des Strahlungsproblems. *Physikalische Zeitschrift* 10: 185–193. Reprinted in facsimile as Doc. 56 in (Einstein, 1987–2006, Vol. 2).
- Einstein, A. (1909b). Über die Entwicklung unserer Anschauungen über das Wesen und die Konstitution der Strahlung. *Deutsche Physikalische Gesellschaft. Verhandlungen* 11: 482–500. Reprinted in facsimile as Doc. 60 in (Einstein, 1987–2006, Vol. 2).
- Einstein, A. (1914). Zum gegenwärtigen Stande des Problems der spezifischen Wärme. Pp. 330–352 in: Arnold Eucken, ed., *Die Theorie der Strahlung und der Quanten*. Halle an der Saale: Knapp. Reprinted in facsimile as Doc. 26 in (Einstein, 1987–2006, Vol. 3).

## Jordan's Resolution of the Conundrum of Wave-Particle Duality of Light

- Einstein, A. (1917). Zur Quantentheorie der Strahlung. *Physikalische Zeitschrift* 18: 121–128. English translation in (Van der Waerden, 1968, pp. 63–77).
- Einstein, A. (1925). Bemerkung zu P. Jordans Abhandlung “Zur Theorie der Quantenstrahlung.” *Zeitschrift für Physik* 31: 784–785.
- Einstein, A. (1987–2006). *The collected papers of Albert Einstein*. 10 Vols. Edited by J. Stachel *et al.* Princeton: Princeton University Press.
- Fölsing, A. (1997). *Albert Einstein. A biography*. New York: Viking.
- Fürth, R. (1928). Über Strahlungsschwankungen nach der Lichtquantenstatistik. *Zeitschrift für Physik* 50: 310–318.
- Gonzalez, J. J. and Wergeland, H. (1973). Einstein-Lorentz formula for the fluctuations of electromagnetic energy. *Det Kongelige Norske videnskabers selskab. Skrifter* 4: 1–4.
- Heisenberg, W. (1925). Über die quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen. *Zeitschrift für Physik* 33: 879–893. Page references to English translation in (Van der Waerden, 1968, pp. 261–276).
- Heisenberg, W. (1926). Schwankungserscheinungen und Quantenmechanik. *Zeitschrift für Physik* 40: 501–506.
- Heisenberg, W. (1930). *The physical principles of the quantum theory*. Chicago: University of Chicago Press.
- Heisenberg, W. (1931). Über Energieschwankungen in einem Strahlungsfeld. *Berichte über die Verhandlungen der Sächsischen Akademie der Wissenschaften zu Leipzig, mathematisch-physikalische Klasse* 83: 3–9.
- Heisenberg, W., and Pauli, W. (1929). Zur Quantendynamik der Wellenfelder. *Zeitschrift für Physik* 56: 1–61.
- Heisenberg, W., and Pauli, W. (1930). Zur Quantendynamik der Wellenfelder, II. *Zeitschrift für Physik* 59: 168–190.
- Hoffmann, D., Ehlers, J., and Renn, J. eds. (2007). *Pascual Jordan (1902–1980). Mainzer Symposium zum 100. Geburtstag*. Max Planck Institute for History of Science, Preprint 329.
- Hoffmann, D., and Walker, M. (2007). Der gute Nazi: Pascual Jordan und das dritte Reich. In (Hoffmann *et al.*, 2007, pp. 83–112).
- Janssen, M., ed. (2006). *Studies in History and Philosophy of Modern Physics*. 37: 1–242 (Special issue—2005: The centenary of Einstein's *annus mirabilis*).
- Jordan, P. (1924). Zur Theorie der Quantenstrahlung. *Zeitschrift für Physik* 30: 297–319.
- Jordan, P. (1925). Über das thermische Gleichgewicht zwischen Quantenatomen und Hohlraumstrahlung. *Zeitschrift für Physik* 33: 649–655.

- Jordan, P. (1927a). Die Entwicklung der neuen Quantenmechanik. *Die Naturwissenschaften* 15: 614–623.
- Jordan, P. (1927b). Die Entwicklung der neuen Quantenmechanik. Schluß. *Die Naturwissenschaften* 15: 636–649.
- Jordan, P. (1927c). Über Wellen und Korpuskeln in der Quantenmechanik. *Zeitschrift für Physik* 45: 766–775.
- Jordan, P. (1928). Die Lichtquantenhypothese. Entwicklung und gegenwärtiger Stand. *Ergebnisse der exakten Naturwissenschaften* 7: 158–208.
- Jordan, P. (1929). Der gegenwärtige Stand der Quantenelektrodynamik. *Physikalische Zeitschrift* 30: 700–713.
- Jordan, P. (1936). *Anschauliche Quantentheorie. Eine Einführung in die moderne Auffassung der Quantenerscheinungen*. Berlin: Julius Springer.
- Jordan, P. (1969). *Albert Einstein. Sein Lebenswerk und die Zukunft der Physik*. Frauenfeld und Stuttgart: Huber & CoAG.
- Jordan, P. (1973). Early years of quantum mechanics: some reminiscences. In (Mehra, 1973, pp. 294–299).
- Jordan, P., and Klein, O. (1927). Zum Mehrkörperproblem der Quantentheorie. *Zeitschrift für Physik* 45: 751–765.
- Jordan, P., and Pauli, W. (1928). Zur Quantenelektrodynamik ladungsfreier Felder. *Zeitschrift für Physik* 47: 151–173.
- Jordan, P., and Wigner, E. (1928). Über das Paulische Äquivalenzverbot. *Zeitschrift für Physik* 47: 631–651.
- Klein, M. J. (1959). Ehrenfest's contributions to the development of quantum statistics. *Proceedings of the Koninklijke Nederlandse Akademie van Wetenschappen. Series B. Physical sciences* 62: 41–50, 51–62.
- Klein, M. J. (1963). Einstein's first paper on quanta. *The Natural Philosopher* 2: 59–86.
- Klein, M. J. (1964). Einstein and the wave-particle duality. *The Natural Philosopher* 3: 1–49.
- Klein, M. J. (1970). The first phase of the Bohr-Einstein dialogue. *Historical Studies in the Physical Sciences* 2: 1–39.
- Klein, M. J. (1979). Einstein and the development of quantum physics. Pp. 133–151 in: A. P. French, ed., *Einstein. A centenary volume*. Cambridge, MA: Harvard University Press.
- Klein, M. J. (1980). No firm foundation: Einstein and the early quantum theory. In (Woolf, 1980, pp. 161–185).

## Jordan's Resolution of the Conundrum of Wave-Particle Duality of Light

- Klein, M. J. (1982). Fluctuations and statistical physics in Einstein's early work. Pp. 39–58 in: G. Holton and Y. Elkana, eds, *Albert Einstein. Historical and cultural perspectives*. Princeton: Princeton University Press. (Reprinted: New York: Dover, 1992.)
- Kojevnikov, A. (1990). Einshteinovskaya formula fluktuatsii i korpuskulyarno-volnovoy dualizm. Pp. 49–97 in: I. Yu. Kobzarev and G. E. Gorelik, eds., *Einshteinovskiy Sbornik, 1986–1990*. Moscow: Nauka. Translation, Einstein's fluctuation formula and the wave-particle duality, in (Balashov and Vizgin, 2002, pp. 181–228).
- Kuhn, T. S., Heilbron, J. L., Forman, P., and Allen, L. (1967). *Sources for the history of quantum physics. An inventory and report*. Philadelphia: American Philosophical Society.
- Kundt, W. (2007). Jordan's "excursion" into geophysics. In (Hoffmann *et al.*, 2007, 123–131)
- Lorentz, H. A. (1916). *Les théories statistiques en thermodynamique: conférences faites au Collège de France en novembre 1912*. Leipzig, Berlin: Teubner.
- Mehra, J., ed. (1973). *The physicist's conception of nature*. Dordrecht: Reidel.
- Mehra, J., and Rechenberg, H. (1982–2001). *The historical development of quantum theory*. 6 Vols. New York, Berlin: Springer.
- Miller, A. I. (1994). *Early quantum electrodynamics. A source book*. Cambridge: Cambridge University Press.
- Milonni, P. W. (1981). Quantum mechanics of the Einstein-Hopf model. *American Journal of Physics* 49: 177–184.
- Milonni, P. W. (1984). Wave-particle duality of light: A current perspective. Pp. 27–67 in: S. Diner, D. Fargue, G. Lochak, and F. Selleri, eds., *The wave-particle dualism: A tribute to Louis de Broglie on his 90th birthday* Dordrecht: Reidel.
- Norton, J. D. (2006). Atoms, entropy, quanta: Einstein's miraculous argument of 1905. In (Janssen, 2006, 71–100).
- Pais, A. (1979). Einstein and the quantum theory. *Reviews of Modern Physics* 51: 863–914.
- Pais, A. (1980). Einstein on particles, fields, and the quantum theory. In (Woolf, 1980, pp. 197–251).
- Pais, A. (1982). 'Subtle is the Lord ...' *The science and the life of Albert Einstein*. Oxford: Oxford University Press.
- Pais, A. (1986). *Inward bound. Of matter and forces in the physical world*. Oxford: Clarendon.
- Pauli, W. (1926). Über das Wasserstoffspektrum vom Standpunkt der neuen Quantenmechanik. *Zeitschrift für Physik* 36: 336–363. English translation in (Van der Waerden, 1968, pp. 387–415).

- Pauli, W. (1930). Review of (Born and Jordan, 1930). *Die Naturwissenschaften* 18: 602.
- Pauli, W. (1979). *Scientific correspondence with Bohr, Einstein, Heisenberg a.o. Volume I: 1919–1929*. Edited by A. Hermann, K. von Meyenn, and V. F. Weisskopf. Berlin: Springer.
- Peierls, R. E. (1973). The development of quantum field theory. In (Mehra, 1973, pp. 370–379).
- Rynasiewicz, R., and Renn, J. (2006). The turning point for Einstein's *annus mirabilis*. In (Janssen, 2006, 5–35).
- Schroer, B. (2007). Pascual Jordan, biographical notes, his contributions to quantum mechanics and his role as a protagonist of quantum field theory. In (Hoffmann *et al.*, 2007, pp. 47–68).
- Schweber, S. S. (1993). Changing conceptualization of renormalization theory. Pp. 137–166 in: L. M. Brown, ed., *Remormalization: From Lorentz to Landau (and Beyond)*. New York: Springer.
- Schweber, S. S. (1994). *QED and the men who made it: Dyson, Feynman, Schwinger, and Tomonaga*. Princeton: Princeton University Press.
- Schwinger, J., ed. (1958). *Selected papers on quantum electrodynamics*. New York: Dover.
- Schwinger, J. (1973). A report on quantum electrodynamics. In (Mehra, 1973, pp. 412–413).
- Smekal, A. (1926). Zur Quantenstatistik der Hohlraumstrahlung und ihrer Wechselwirkung mit der Materie. *Zeitschrift für Physik* 37: 319–341.
- Stachel, J. (1986). Einstein and the quantum. Fifty years of struggle, pp. 349–385 in: R. G. Colodny, ed., *From quarks to quasars. Philosophical problems of modern physics*. Pittsburgh: University of Pittsburgh Press. Page references to reprint in (Stachel, 2002, pp. 367–402).
- Stachel, J. (2002). *Einstein from 'B' to 'Z'*. Boston: Birkhäuser.
- Uffink, J. (2006). Insuperable difficulties: Einstein's statistical road to molecular physics. In (Janssen, 2006, 36–70).
- Van der Waerden, B. L., ed. (1968). *Sources of quantum mechanics*. New York: Dover.
- Van Dongen, J. (2007a). Emil Rupp, Albert Einstein, and the canal ray experiments on wave-particle duality: Scientific fraud and theoretical bias. *Historical Studies in the Physical and Biological Sciences* 37 (Supplement): 73–120.
- Van Dongen, J. (2007b). The interpretation of the Einstein-Rupp experiments and their influence on the history of quantum mechanics. *Historical Studies in the Physical and Biological Sciences* 37 (Supplement): 121–131.

## Jordan's Resolution of the Conundrum of Wave-Particle Duality of Light

- Von Meyenn, K. (2007). Jordan, Pauli, und ihre frühe Zusammenarbeit auf dem Gebiet der Quantenstrahlung. In (Hoffmann *et al.*, 2007, pp. 37–46).
- Weinberg, S. (1977). The search for unity: notes for a history of quantum field theory. *Daedalus* 106: 17–35.
- Weinberg, S. (1995). *The quantum theory of fields*. Vol. 1. *Foundations*. Cambridge: Cambridge University Press.
- Wentzel, G. (1960). Quantum theory of fields (until 1947), pp. 48–77 in: M. Fierz and V. F. Weisskopf (eds.), *Theoretical physics in the twentieth century. A memorial volume to Wolfgang Pauli*. New York: Interscience Publishers. Reprinted in (Mehra, 1973, pp. 380–403).
- Wightman, A. S. (1996). How it was learned that quantized fields are operator-valued distributions. *Fortschritte der Physik* 44: 143–178.
- Wolfke, M. (1921). Einsteinsche Lichtquanten und räumliche Struktur der Strahlung. *Physikalische Zeitschrift* 22: 375–379.
- Woolf, H., ed. (1980). *Some strangeness in the proportion. A centennial symposium to celebrate the achievements of Albert Einstein*. Reading, MA: Addison-Wesley.



# 11 Why Were Two Theories Deemed Logically Distinct, and Yet, Equivalent in Quantum Mechanics?

SLOBODAN PEROVIC

*A recent rethinking of the early history of Quantum Mechanics deemed the late 1920s agreement on the equivalence of Matrix Mechanics and Wave Mechanics, prompted by Schrödinger's 1926 proof, a myth. Schrödinger supposedly failed to achieve the goal of proving isomorphism of the mathematical structures of the two theories, while only later developments in the early 1930s, especially the work of mathematician John von Neumann (1932) provided sound proof of equivalence. The alleged agreement about the Copenhagen Interpretation, predicated to a large extent on this equivalence, was deemed a myth as well.*

*If such analysis is correct, it provides considerable evidence that, in its critical moments, the foundations of scientific practice might not live up to the minimal standards of rigor, as such standards are established in the practice of logic, mathematics, and mathematical physics, thereby prompting one to question the rationality of the practice of physics.*

*In response, I argue that Schrödinger's proof concerned primarily a domain-specific ontological equivalence, rather than the isomorphism. It stemmed initially from the agreement of the eigenvalues of Wave Mechanics and energy-states of Bohr's Model that was discovered and published by Schrödinger in his First and Second Communications of 1926. Schrödinger demonstrated in this proof that the laws of motion arrived at by the method of Matrix Mechanics could be derived successfully from eigenfunctions as well (while he only outlined the reversed derivation of eigenfunctions from Matrix Mechanics, which was necessary for the proof of isomorphism of the two theories). This result was intended to demonstrate the domain-specific ontological equivalence of Matrix Mechanics and Wave Mechanics, with respect to the domain of Bohr's atom. And although the full-fledged mathematico-logical equivalence of the theories did not seem out of the reach of existing theories and methods, Schrödinger never intended to fully explore such a possibility in his proof paper. In a further development of Quantum Mechanics, Bohr's complementarity and Copenhagen Interpretation captured a more substantial convergence of the subsequently revised (in light of the experimental results) Wave and Matrix Mechanics.*

*I argue that both the equivalence and Copenhagen Interpretation can be deemed myths if one predicates the philosophical and historical analysis on a narrow model of physical theory which disregards its historical context, and focuses exclusively on its formal aspects and the exploration of the logical models supposedly implicit in it.*



## Introduction<sup>1</sup>

Recently, based on a careful scrutiny of the key arguments pursued by physicists at the beginning of the Quantum Revolution, several philosophers have characterized some of the essential agreements between these physicists as unsubstantiated and unjustified.

To cite perhaps the most notable example, in the late 1920s, the community of quantum physicists agreed on the equivalence of the two competing formal accounts of quantum phenomena, namely, V. Heisenberg's Matrix Mechanics and E. Schrödinger's Wave Mechanics.

Early on, these accounts had been perceived to be substantially different in terms of the mathematical techniques they employed. The Matrix Mechanics was an algebraic approach employing the technique of manipulating matrices. The Wave Mechanics, in contrast, employed differential equations and had a basic partial differential wave equation at its heart.

In addition, the formalisms were initially applied to *two distinct sets of experimental results*. The Matrix Mechanics was deemed successful in treating the appearance of spectral lines and later was found to be successful (to some extent) in experiments with electron scattering. For the Wave Mechanics, its initial applicability to light interference experiments was extended to include the account of the energy values in experiments with hydrogen atoms.

And finally, the ontological commitments arising from the formalisms were at odds with each other. Heisenberg's approach stressed the discrete properties of the observed phenomena, such as the occurrence of spectral lines of different intensities, and attempted to reduce them to essentially corpuscular properties. Schrödinger perceived the field-like continuity of some key micro-physical phenomena (e.g., those related to the double-slit experiments), as they were accounted for by Wave Mechanics, as its main advantage over the old quantum mechanics.

It is not easy to determine to what extent each of these contrasting aspects was responsible for the general understanding that the two theories were irreconcilable. Be that as it may, because of this widespread belief, when the argument for their supposed equivalence was first conceptualized and published by Schrödinger in 1926, it was seen as a major breakthrough—it predicated the development of quantum mechanics.

Recently, however, F.A. Muller (1997a, 1997b) has deemed this equivalence a myth. Muller argues that the initial agreement concerning the equivalence was based on the misconception that both empirical and mathematical equivalence were successfully demonstrated, and that only later developments in the early 1930s, especially the work of mathematician John von Neumann (1932), provided sound proof of the mathematical equivalence, as opposed to the more famous proof provided by Schrödinger or similar attempts by others (Eckart; Dirac; Pauli).

If this re-evaluation tells the true story, it implies that the wide agreement among physicists on the equivalence of two formalisms in the 1920s, on which further developments of the theory were critically predicated, was an unjustified, indeed, an irrational act of faith (or myth, as Muller labels it) on the part of the physics community.

Even the so-called Copenhagen Interpretation of Quantum Mechanics, which has dom-

---

<sup>1</sup>A revised version of this work is forthcoming in the 2008 April volume of *Studies in History and Philosophy of Science Part B: Studies in History and Philosophy of Modern Physics*.

## Why Were Two Theories Deemed Logically Distinct, Yet Equivalent?

---

inated the field since the 1930s, *and which stemmed from the new Quantum Mechanics, largely predicated on the alleged equivalence*, was debunked by the same rethinking of the history of the debate over the foundations of quantum theory (Beller, 1999), and was deemed another myth (Howard, 2004). Thus, presumably, the agreement on the interpretation that argued for the synthesis predicated on both the Wave Mechanics and Matrix Mechanics (initially Niels Bohr's interpretation), and which was thought to have had successfully countered the arguments for the exclusive commitment to continuity based on Wave Mechanics on the one hand, and the discontinuity based on Matrix Mechanics on the other, was forced on the community by the Göttingen group (Beller, 1999) and/or constructed as a myth by subsequent deliberate or semi-deliberate misinterpretations of the history (Howard, 2004). In any case, focusing on the agreement on the mathematico-logical equivalence favors such views. If the mathematico-logical equivalence (i.e., isomorphism) of the two theories was proved in the 1920s, then the physical theory as such did not favor Copenhagen Interpretation over the other two interpretations (Schrödinger's and Heisenberg's), at least not in any straightforward way. But then it becomes rather puzzling how could have such a wide agreement on the Copenhagen Interpretation been justified (if the agreement was reached at all). And if the agreement on the mathematico-logical equivalence was unjustified, as Muller claims, the distinctness of the competing theories could hardly offer a powerful argument for the Copenhagen Interpretation, that won overwhelmingly against the arguments for both wave-mechanical and matrix mechanical approach.

If such analysis is correct, it provides considerable evidence that, in its critical moments, the foundations of scientific practice might not live up to even minimal standards of rigor, as such standards are established in the practice of logic, mathematics, and mathematical physics, thereby prompting one to question the rationality of the practice of physics. Following Muller's line of attack, one might argue that only the efforts of a few able logicians, mathematicians, and mathematical physicists, keen on developing rigorous mathematical models of phenomena, and logical analysis of such models, have a chance of saving science from this charge of (possibly unavoidable) malpractice and messy development predicated on myths and unjustified agreements. Perhaps only in rare moments of lucidity, thanks to these champions of rationality, can we find commendable rational principles at work in science. Furthermore, those pursuing philosophical concerns about the nature of the physical world should draw their insights exclusively from the theory as it is defined at such rare moments.

So did the philosophers finally get it right, or have they missed something crucial in their analysis of scientific practice in the case of Quantum Mechanics? I will argue the latter.

More specifically, I will argue that rationality in physics, and possibly in science more generally, appears elusive in the key moments (and consequently, the rational pursuit essentially is exclusively reserved for the abstraction of logical modeling and the analysis of natural phenomena), only if we premise our analysis of actual scientific practice on narrow models of scientific knowledge. These models, such as that of P. Suppes (1957, 1960), used in the above-outlined analysis of the equivalence case, reduce the conceptual and historical analysis to the aspects of scientific knowledge having to do with the mathematical-logical analysis of the formalisms (such as Matrix Mechanics and Wave Mechanics), which, although indispensable in some aspects of scientific practice, may not

be necessary in the establishment of its rational procedures. Such a narrowly-focused analysis is bound to miss some key aspects of the physicists' arguments, embedded as they are in historical and philosophical contexts, contexts which must be unraveled if one is to do justice to the physicists' thinking.

With respect to equivalence, I will argue that the kind of equivalence pursued at a later stage by Von Neumann, and which allegedly represents a moment of lucidity in the overwhelming messiness of the development of Quantum Mechanics, was a very narrowly focused refinement of the previous agreement on the initial concept of equivalence. Although it is true that Schrödinger failed to provide a full-fledged proof of logical equivalence, for the reasons that Muller points out, his paper contained only a preliminary attempt to do so.

Judging by its structure, its content, and the historical context in which it appeared, *Schrödinger's proof concerned a domain-specific ontological equivalence, the domain being Bohr's atom*. Bohr's complementarity and Copenhagen Interpretation captured a more substantial convergence of, the subsequently revised (in light of the experimental results), theories. Furthermore, even the full-fledged logical equivalence of the theories did not seem out of the reach of the existing theories and methods, although Schrödinger never intended to fully explore such a possibility in his proof paper.

## The Alleged Myth of the Equivalence

Muller (1997a, 36) argues, "The Equivalence Myth is that matrix mechanics and wave mechanics were mathematically and empirically equivalent at the time when the equivalence proofs appeared and that Schrödinger (and Eckart) demonstrated their equivalence" (although Schrödinger's proof was more elaborate and influential than Eckart's). Thus, the argument goes, Schrödinger (1926a) attempted to prove the mathematical equivalence of Matrix Mechanics and Wave Mechanics by demonstrating their *isomorphism* (the *explanans* of Schrödinger's overall argument), in order to explain their allegedly established empirical equivalence (*explanandum*) (Muller 1997a, 49). Yet, Muller argues, contrary to the widespread belief at the time (and subsequently), Wave Mechanics and Matrix Mechanics were neither proven mathematically equivalent by Schrödinger, nor were they empirically equivalent.

The incorrect view that Wave Mechanics and Matrix Mechanics were empirically equivalent, Muller argues, stems from an overlooked fact that the two could and should have been treated as empirically distinct in light of the available knowledge. That the electron charge densities were smeared was overlooked, and this "made it conceivable to perform an *experimentum crucis* by charge density measurements" (Muller 1997a, 38) Moreover, the empirical agreement between Wave Mechanics and Matrix Mechanics hinted at by Schrödinger (1926a) on the first page of his paper concerns two cases that are insufficient as evidence of the purported empirical equivalence. The first case was a rather tenuously relevant (to the empirical equivalence thesis) case of coinciding energy values for the hydrogen atom and "the few toy systems" (Muller 1997a, 49), and the second was the quantisation of orbital angular momentum. I will say more about both cases shortly.

If Schrödinger's goal was to prove isomorphism of Wave Mechanics and Matrix Mechanics, the equivalence at stake should be characterized as mathematico-logical equiva-

lence, since labeling it merely ‘mathematical equivalence’ could refer to the employment of mathematical techniques have no clear logical pretensions or consequences.<sup>2</sup> Muller’s idea of the equivalence at stake is much stronger than this. He states that since “the essence of a physical theory lies in the mathematical structures it employs, to describe physical systems, the equivalence proof, including part of Schrödinger’s intentions, can legitimately be construed as an attempt to demonstrate the isomorphism between the mathematical structures of matrix mechanics and wave mechanics” (Muller 1997a, 38).

There are three different reasons for the supposed failure of the mathematico-logical (or let us call it simply logical) equivalence. The first reason is that the absence of a state-space in Matrix Mechanics prevented the *direct mutual translation of sentences of Wave Mechanics and Matrix Mechanics*. A related second reason is that the language of Matrix Mechanics could not refer to space, charge-matter densities, or eigenvibrations,<sup>3</sup> “because Matrix Mechanics did not satisfy (in the rigorous model-theoretic sense) any sentence containing terms or predicates referring to these notions” (Muller 1997a, 39). Finally, the most substantial reason was the failure of what Muller labels “Schrödinger-equivalence”—an attempted (Muller believes) proof of a “softer” equivalence than the related one which required a full-fledged logical proof—a failure which was due to the unjustified assumptions regarding the so-called “the problem of the moments” of a function (and this was allegedly resolved in Von Neumann’s proof). (Muller 1997b)

### The Empirical Evidence in Early Quantum Mechanics

But was there really a myth of *empirical equivalence*? If so, was it an explanandum of Schrödinger’s overall argument?

It is hard to argue for the existence of such a myth without assuming an oversimplified portrayal of the relevance of empirical evidence in the early days of Quantum Mechanics. Schrödinger’s (1926a, 45) expression concerning the agreement “with each other” of Wave Mechanics and Matrix Mechanics “with regard to the known facts,” employed at the beginning of his proof paper, reflects, at least in Muller’s view, the claim of the full-blown empirical agreement.<sup>4</sup> This is a convenient characterization if one aims at constructing the full-fledged empirical equivalence as an explanandum of Schrödinger’s (supposed) overall explanation. It is then easy to demonstrate its failure, as Muller does, for example, by pointing to the incapability of Wave Mechanics to account for the line intensities. (Muller 1997a, 54)

But the expression could also reflect the view that although there was some compelling agreement between the two, it was not firmly established. As such, it was not the only, or perhaps the decisive motive for devising the proof. In fact, Schrödinger never committed himself to a strong view of empirical equivalence, and it is actually very unlikely that

---

<sup>2</sup>Schrödinger’s statements about “mathematical equivalence” are ambiguous. See footnote 10.

<sup>3</sup>See the explanation of eigenvibrations on pp. 16–17.

<sup>4</sup>It turns out, as I will argue later on, that in order to properly analyze this Schrödinger’s statement, the passage should be read in its entirety. “Considering the extraordinary differences between the starting-points and the concepts of Heisenberg’s quantum mechanics and of the theory which has been designated “undulatory” or “physical” mechanics, and has lately been described here, it is very strange that these two new theories agree *with one another* with regard to the known facts, where they differ from the old quantum theory. I refer, in particular, to the peculiar “half-integralness” which arises in connection with the oscillator and the rotator.” (1926a, 45)

anybody else believed in the full-blown empirical equivalence at the time.

As a matter of fact, some experiments were considered crucial, as they were conceived and performed to decide between the opposing views of micro-physical systems. A set of such experiments concerned the problem of smeared charge densities, the (alleged) lack of which is cited by Muller as evidence of unjustified agreement on the empirical equivalence.

Schrödinger's early wave-mechanical treatment of the atom as a charge cloud (instead of an electron as a particle, orbiting around the nucleus—Bohr's early model) did not at first accurately account for radiation of the atom (while Bohr's model did), given that only certain energy states were observed in spectroscopic experiments. The electric density of the cloud differed from place to place but remained permanent. Thus, in order to account for the radiation in corresponding energy states of the atom, Schrödinger introduced the idea of vibrations of the charge cloud in two or more different modes with different frequencies (i.e., the eigenvibrations accounted for by eigenvalues of the wave equation). As a consequence, the radiation is emitted in the form of *wave-packets* of only certain energies, corresponding to Bohr's frequency conditions. Since Schrödinger assumed that the classical electromagnetic theory accounts for the atom radiation, a number of different radiations could be emitted by the atom as the wave-packet of certain energy expands in space.<sup>5</sup> In the introduction to his proof, Schrödinger (1927a, 45) refers to the case of the oscillator, a special case of this Wave Mechanics treatment of radiation.<sup>6</sup>

The consequences of Schrödinger's theory, which contradicted Bohr's early view of radiation, were probed experimentally by a series of crucial experiments (Compton and Simon, 1925; Bother and Geiger, 1926).<sup>7</sup> Thus, at the time of writing the proof paper, Schrödinger, as well as others, knew that despite the initial agreement of his theory with Bohr's results with respect to the energy states and radiation, the issue could be addressed further by directly probing "individual radiation processes" that would, in turn, indirectly test the plausibility of the assumption about the vibrations of the atom. Schrödinger was cautioned but was not entirely convinced until 1927 (Mehra and Rechenberg 1982, 138) that the results of these new experiments unequivocally demonstrated the discontinuous nature of matter-energy micro-interactions, as Bohr had claimed. Thus, the issue had been addressed experimentally but remained unresolved at the time of the appearance of the proof.

Nor could the experiments concerning the related issue of quantisation of the orbital angular momentum (referred to as the 'rotator case' by Schrödinger at the beginning of the paper (1927a, 45)) have contributed to the presumed (by Muller) agreement on the empirical equivalence. By introducing the quantised angular momentum of electron, Bohr's model predicted correctly the spectral lines (i.e., Balmer lines) that corresponded to the allowed rotational frequencies of the electron. Heisenberg started with the discrete values of the spectral lines and developed matrices accounting for them. Schrödinger admitted (1926b, 30) that his Wave Mechanics was not capable of accounting for Balmer lines as straightforwardly as Matrix Mechanics did. Yet he presumed this to be a mere

---

<sup>5</sup>Perhaps surprisingly, this assumption was not at odds with what Bohr believed shortly before Schrödinger developed his own view, as Bohr was advocating the Bohr-Kramers-Slater theory that made a very similar assumption about the way the atom radiated energy.

<sup>6</sup>See footnote 3.

<sup>7</sup>See also (Stuewer, 1975) and (Perovic, 2006).

## Why Were Two Theories Deemed Logically Distinct, Yet Equivalent?

---

technical advantage (Schrödinger 1926a, 57), and the equivalence proof set out to demonstrate this. Schrödinger doubted (and offered his reasons in the proof for this doubt) that this particular success of Heisenberg's approach necessarily reflected a substantial (epistemological or ontological) advantage of Matrix Mechanics, as it was not clear whether the spectral lines indicated the nature of *individual* corpuscular-like interactions of radiation with the matter (i.e., with the spectroscopy), or whether they were the consequence of the way wave-packets, not individual corpuscles, interacted with the matter. This issue was also addressed by the above-mentioned scattering experiments and earlier by Ramsauer's (1921) experiments.

The experiments in these two cases, although perceived to be crucial by both the experimentalists (Compton) and those interested in their theoretical implications, did not immediately prompt discarding either approach, if for no other reason than the physicists were simply unsure at the time, how exactly to apply the newly developed formalisms to particular experiments (Heisenberg in Mehra and Rechenberg, 1982, 151). Even a superficial look at the correspondence among them shows that they continued discussing the application of the formalisms and the meaning of such application well into the late 1920s.

Also, it is misleading to say that the coinciding energy values for the hydrogen atom and “a few toy systems,” as Muller calls them, were perceived as key evidence of the empirical equivalence of Matrix Mechanics and Wave Mechanics. In fact, these “toy systems” were directly based on Bohr's model of the atom, and Schrödinger's initial major interest concerned the agreement between energy values arrived at by Wave Mechanics (Schrödinger, 1926b; 1926c) and those predicted by Bohr's theory. (Jammer, 1989, 275) This agreement prompted Schrödinger to think about the connection with Heisenberg's Matrix Mechanics. Therefore, the initial agreement between Bohr's model and Schrödinger's Wave Mechanics, that I will discuss shortly, is an essential element of the motivation for the proof.

All these considerations were on going while Schrödinger and others were devising their proofs. More importantly, neither Schrödinger nor anybody else was certain whether or to what extent either of the two formalisms fully accounted for the observed properties of micro-physical processes, *nor whether either was indispensable*. As Jammer (1989, 210) puts it, Matrix Mechanics and Wave Mechanics were “designed to cover the same range of experiences” but it was not firmly established in 1926 that either did so.

Thus, there was considerable agreement with the facts of Wave Mechanics and Matrix Mechanics. This prompted the question about the possibility of a substantial equivalence (both empirical and mathematical). This, in turn, encouraged the construction of new crucial experiments, pushing the limits of the applicability of existing formalisms to them. Given this, the use of the phrase “the two new theories agree with one another with regard to the known facts” was a conditional statement—as both the continuation of the sentence (“where they [Wave Mechanics and Matrix Mechanics] differ from the old quantum theory”), and the subsequent sentence (which tempers the claim by revealing a clearly theoretical consideration behind the mention of the factual connection)<sup>8</sup> indicate.<sup>9</sup> The intention was much more tenuous than the full-fledged empirical evidence demands. And the motivation for the proof (or explanandum) should not be reduced to the meaning

---

<sup>8</sup>See footnote 14.

<sup>9</sup>See the entire sentence in the footnote 3.

of the phrase treated independently from the context of both the proof paper and the experimental and theoretical knowledge of the time. What Schrödinger had in mind was not a ‘myth’ of full-fledged empirical equivalence that should be explained. Rather, he wished to show that the factual state of affairs indicated the possibility of domain-specific equivalence, stemming from the agreement of eigenvalues and Bohr’s energy levels, as we will see shortly, which could be revealed by fairly simple manipulations of both methods.

## Was Schrödinger’s Proof a Proof of Logical Equivalence?

It is tempting to define the goal of Schrödinger’s proof as a single goal. Although there might be a single most important goal, the text reveals the complexity and hierarchy of Schrödinger’s intentions.<sup>10</sup>

In a passage that precedes the actual proof, Schrödinger states that “[i]n what follows the very intimate *inner connection* between Heisenberg’s quantum mechanics and my wave mechanics will be disclosed” (Schrödinger, 1926a, 46). He continues, “From the formal mathematical standpoint, one might well speak of the *identity* of the two theories” and concludes the paragraph by saying, “The train of thought in the proof is as follows.”

An initial reading of this passage might suggest that the author is about to provide a full-blown mathematico-logical proof and that one should judge the effort based on this assumption. Even if Schrödinger’s intentions were different, or at least diverse in terms of the proof’s goals, the mention of the equivalence from “the mathematical standpoint” might urge one to accept such a narrow interpretation. It is possible, however, and as I will argue, quite likely that a rather different key goal is referred to by another phrase used in the passage, namely, the reference to “the intimate connection” between Matrix Mechanics and Wave Mechanics, and that the *subsequent* phrase, “mathematical standpoint,” refers to a distinct issue treated separately in the proof.

We should certainly not rely on this one passage. It does not help, though, that another passage that mentions the goals and the nature of the proof is also quite ambiguous (Schrödinger 1926a, 57–58).<sup>11</sup> Nor does it help that Schrödinger’s attitude with regards to proving the equivalence appears to change significantly over time. In a letter to Wien, dated March 1926, he writes that “both representations are—from the purely mathematical point of view—totally equivalent.” (Mehra and Rechenberg, 1982, 640) Yet in his second Communication, he states that Matrix Mechanics and Wave Mechanics “will supplement each other” (Schrödinger, 1926c, 30)<sup>12</sup> pointing out the advantages of each over the other, rather than noting their similarities. Moreover, as Jammer (1982, 273) points out, the physical and mathematical equivalences that Schrödinger (1926a, 58) mentions, are quite possibly distinct, although we can hardly determine, based on

---

<sup>10</sup>A similar complexity can be revealed in other proofs devised at the time as well.

<sup>11</sup>His adamant statement that “they are completely equivalent from the mathematical point of view, and it can only be a question of the subordinate point of convenience of calculation” (p. 57) certainly overstates the case as the passages that follow this sentence suggest a much more moderate discussion of the formalisms and only a preliminary discussion of logical equivalence. In this context, it is hard to see how the phrase could be interpreted to refer to the isomorphism.

<sup>12</sup>“I am distinctly hopeful that these two advances will not fight against one another, but on the contrary, just because of the extraordinary difference between the starting-points and between methods, that they will supplement one another and that the one will make progress where the other fails.” (Schrödinger, 1926c, 30)

## Why Were Two Theories Deemed Logically Distinct, Yet Equivalent?

---

the text of the proof alone, whether or to what extent Schrödinger believed this and what exactly such a view would imply.

A textual analysis of the relevant passages that explicitly state the goals of the proof, although necessary, can go only so far. In order to determine, first, what the real intentions, and possible achievements, of the proof were, and second, how they were perceived by others, we must judge the text within the historical context in which it was written.

The proof was not motivated by empirical considerations alone. Possibly more important was agreement with Bohr's model of the atom. It prompted articulation of the key step in the proof: the construction of matrices based on the eigenfunctions. As Gibbins says, "Schrödinger in 1926 proved the two theories... equivalent," albeit ontologically, not empirically, "*at least as far as the stationary, or stable-orbit, values for dynamical variables were concerned*" (Gibbins, 1987, 24).

As a matter of fact, both Matrix Mechanics and Wave Mechanics were constructed against the background of Bohr's model and were attempts to improve and, finally, to replace it. While Bohr's model had been changing since its inception, the importance of stationary (permitted) energy states in understanding quantum phenomena remained intact.<sup>13</sup> And as we will see, it became clear to what extent this core of the model remained insightful once Matrix Mechanics and Wave Mechanics were fully developed and the proofs of their equivalence devised.

Bohr's correspondence rules were indispensable guidelines for the construction of Matrix Mechanics in its early phase. As a matter of fact, Matrix Mechanics was envisioned as an improved version of Bohr's method. From Heisenberg's point of view, after he developed Matrix Mechanics, Bohr's method was a useful, albeit rough, first approximation. Matrix Mechanics emerged as a fully independent method once Heisenberg joined efforts with Born and Jordan (Born, Heisenberg, and Jordan, 1926; Jammer, 1989, 221). Commenting on this, Lorentz optimistically notes in 1927, "The fact that the coordinates, the potential energy, etc., are now represented by matrices shows that these magnitudes have lost their original meaning, and that a tremendous step has been taken towards increasing abstraction." (Lorentz in D'Abro, 1951, 851)

Pauli's application of Matrix Mechanics to the hydrogen atom illustrated the independence of the method in a similar fashion. (Mehra and Rechenberg, 1982, 656–657) Yet Pauli realized that the fundamental assumptions concerning quantum phenomena, as approached from the point of view of Matrix Mechanics, are in agreement with Bohr's model and that, in this sense, the two might not be as different as they are in terms of methodology.

An insight concerning the relation of Wave Mechanics and Bohr's model, very similar to that of Pauli's concerning Matrix Mechanics, motivated Schrödinger to write the proof paper. In order to understand this, it is critical to take into account that the agreement of Wave Mechanics and Bohr's model (i.e., its core concerning stationary states) precedes the agreement of Wave Mechanics and Matrix Mechanics.

If one replaces the parameter  $E$  in Schrödinger's equation

$$\Delta\psi + \frac{8\pi^2m_0}{h^2}[E - E_{pot}(x, y, z)] \psi = 0$$

---

<sup>13</sup>According to Bohr's early model (Bohr, 1913) electrons of the atom can occupy only certain orbital states characterized by appropriate energy levels.



with one of the so-called eigenvalues,  $E_n$ , the equation will have a solution (thus becoming one of the eigenfunctions for a given eigenvalue).<sup>14</sup> The solution determines the amplitude of the de Broglie wave (stemming from his compromise between corpuscular mechanics and the theory involving continuity), while the eigenvalue (i.e., the energy) determines the frequency of the wave—that is, the chosen eigenvalue and the corresponding eigenfunction determine the mode of (eigen) vibration.

Now, Schrödinger's solution of the hydrogen atom eigenvalue equation of his first and second communication of 1926 (Schrödinger, 1926b, 1926c) resulted unexpectedly in Bohr's energy levels. Or more precisely, as Bohr, who understood the importance of the insight, stated in 1927, "The proper vibrations of the Schrödinger wave-equation have been found to furnish a representation of electricity, suited to represent the electrostatic properties of the atom in a stationary state" (Bohr, 1985, V.6, 96).<sup>15</sup>

This insight made a great impression on Schrödinger. The newly discovered agreement raised a deeper question concerning an apparently discontinuous nature of the system imposed on an essentially continuous approach of Wave Mechanics by quantum conditions. Others were equally impressed: Wentzel immediately set out to examine this agreement with a new Wave Mechanics approximation method (Jammer, 1989, 275–276).

Wave Mechanics had already emerged as methodologically independent from Bohr's account, and Schrödinger states this explicitly in the first section of the proof: "... we have a continuous field-like process in configuration space, which is governed by a single partial differential equation, derived from a principle of action. This principle and this differential equation replace the equations of motion and the quantum conditions of the older 'classical quantum theory'." (1926a, 45). *However, in light of this newly obtained agreement, it was not obvious that Wave Mechanics's independence, like that of Matrix Mechanics, was not merely a methodological independence.*

Schrödinger was well aware of all this, and it guided the development of the equivalence proof. The central issue of the proof was ontological, rather than the logical. Arguably, it was an attempt, motivated by Wave Mechanics's agreement with Bohr's model, to demonstrate the ontological significance of Wave Mechanics's assumptions (i.e., their non-*ad hoc* nature), and its epistemological significance, doubted (by Heisenberg and others in the Göttingen school, and perhaps Schrödinger himself at first) because of its inapplicability to the spectral line intensities. In other words, given that *Wave Mechanics and Bohr's model agreed with respect to the eigenvalues and stationary energy states, the*

<sup>14</sup>Mathematically speaking, if a differential equation (such as Schrödinger's equation) contains an undetermined parameter, and it admits solutions only when particular values (eigenvalues or proper values) are assigned to the parameter, the solutions of the equation are called eigenfunctions.

<sup>15</sup>In (1926b, 8) Schrödinger starts from the wave mechanical assumptions and derives the expression  $-E_1 = \frac{m(e^2)^2}{2K^2\hbar^4}$  where "the well known Bohr energy-levels, corresponding to the Balmer lines, are obtained, if the constant  $K$ , introduced in for reasons of dimensions, we give the value  $K = \frac{\hbar}{2\pi}$ , from which comes  $-E_1 = \frac{2\pi^2 m(e^2)^2}{\hbar^2}$ ." In (1926c, 27–28), at the end of the discussion of the case of the rotator, Schrödinger generalizes the expression of an earlier derived wave function ( $\text{div grad } \psi - \frac{1}{u^2} \psi''$ ) in the following way: "For it is possible to generalize by replacing  $\text{div grad } \psi$  by  $f(qk) \text{div}\{[\frac{1}{f(qk)}] \text{grad } \psi\}$ , where  $f$  may be an arbitrary function of the  $q$ 's, which must depend in some plausible way on  $E, V(qk)$ , and the coefficients of the line elements." Later on, he comments on the agreement between energy values in Bohr's theory and eigenvalues (discussed on p. 26), emphasizing the advantage of his approach: "... the quantum levels are at once defined as the proper values of equation (18) [wave equation], which carries in itself its natural boundary conditions." (p. 29) The entire argument for the advantage of the wave-mechanical approach in the second Communication was predicated on this agreement.

question was whether Wave Mechanics and Matrix Mechanics agreed with respect to eigenvalues and, thus, to stationary states as well.

## The Proof of the Domain-Specific Ontological Equivalence—as Far as Eigenvalues/Stationary States Go

Although the above-stated central goal of Schrödinger's proof may seem disappointingly modest, one should bear in mind that the importance of elucidating the nature of the “intimate connection” between Matrix Mechanics and Wave Mechanics was only superficially apparent at the time, and might have been unsuccessful, as the independence of the two theories could have turned out to be more fundamental.<sup>16</sup> In any case, Schrödinger's expression of the “intimate connection” between Matrix Mechanics and Wave Mechanics, rather than his reference to the “mathematical equivalence” of the two, indicates the central goal of the proof. That Schrödinger “compared Wave Mechanics and Matrix Mechanics,” as M. Bitbol (1996, 68) labels the endeavor, was far more important than his attempted mathematico-logical proof.

The very *structure of the proof* is best explained if the proof were intended to offer further insight into the agreement between Bohr's model and Wave Mechanics, by constructing suitable matrices from eigenfunctions, thereby demonstrating the “intimate connection” between Wave Mechanics and Matrix Mechanics, and thus, indirectly showing the (ontological) significance of their agreement with Bohr's (revised) model.<sup>17</sup>

Schrödinger's paper can be divided into four parts—the introduction, which I have just discussed, and the three parts of the actual proof.<sup>18</sup>

*Part 1* of the proof establishes the preliminary connection between Matrix Mechanics and Wave Mechanics. Very early on, Schrödinger emphasizes the limitations placed on his attempt (i.e., quantum conditions). And he explicates the background conditions of the Matrix Mechanics that originate from Bohr's model (i.e., with stationary states and the correspondence rules). He states: “I will first show how to each function of the position and momentum-co-ordinates there may be related a matrix in such a manner, that these matrices, in every case, satisfy the formal calculating rules of Born and Heisenberg (among which I also reckon the so-called ‘quantum condition’ or ‘interchange rule’)” (1926a, 46). (Briefly stated, the idea was that the interchange rules—that were, initially at least, a condition that stemmed from Bohr's model—correspond to the analysis of the linear differential operators used in Wave Mechanics.)

Thus, since Born-Heisenberg's matrix relation  $\mathbf{pq} - \mathbf{qp} = (\frac{\hbar}{2\pi i})\mathbf{1}$  corresponds to the Wave Mechanics relation  $[(\frac{\hbar}{2\pi})(\frac{\partial}{\partial q})]q\psi - q[(\frac{\hbar}{2\pi i})(\frac{\partial}{\partial q})]\psi = (\frac{\hbar}{2\pi i})\psi$ , a differential operator  $F[(\frac{\hbar}{2\pi i})(\frac{\partial}{\partial q}), q]$  can be associated with the function of momentum and position  $F =$

---

<sup>16</sup>Already in (1926c) while discussing the rotator case, he notes the agreement between Matrix Mechanics and Wave Mechanics, with respect to the quantum energy levels: “Considering next the proper values, we get ...  $E_n = \frac{(2n+1)}{2} h\nu_0$ ;  $n = 0, 1, 2, 3, \dots$ . Thus as quantum levels appear so-called “half-integral” multiples of the “quantum of energy” peculiar to the oscillator, i.e. the *odd* multiples of  $\frac{h\nu_0}{2}$ . The intervals between the levels, which alone are important for the radiation, are the same in the former theory. It is remarkable that our quantum levels are *exactly* those of Heisenberg's theory.” (p. 31)

<sup>17</sup>It was almost certainly understood by others this way, as I will argue shortly.

<sup>18</sup>Parts 1 and 2 do not correspond exactly to the original paragraphs of the paper, whereas Part 3 pretty much corresponds to the last paragraph.

$F(p, q)$ . If the phase velocity functions,  $u_k = u_k(q)$ , in the configuration space of the position  $q$  form a complete orthonormal set, then an equation  $F_{jk} = \int u_k^* j[F, u_k] dq$ , can be derived that determines the elements of the matrix  $F_{jk}$ . Thus, as this argument goes, in this very particular sense, any equation of Wave Mechanics can be consistently translated into an equation of Matrix Mechanics.

Part 2 addresses the pressing issue of whether it is possible to establish the “inner connection” between Matrix Mechanics and Wave Mechanics and, hence, the agreement of both with Bohr’s model. This part of the text is the key to the proof, as Schrödinger and others saw it, as it provides the *unidirectional argument for the ontological equivalence* as far Bohr’s atom goes—by constructing suitable matrices from eigenfunctions.

Relying on the insights of Part 1, Schrödinger replaces the  $u_i$  of the  $u_k = u_k(q)$  with the eigenfunctions of his wave equation. Thus, he obtains an operator function:  $[H, \psi] = E\psi$ . The operator’s eigenvalues  $E_k$  satisfy the equation  $[H, \psi_k] = E_k\psi_k$ . As it turns out, solving this equation is equivalent to diagonalizing the matrix  $H$ .<sup>19</sup>

In the *final and decisive step* of Part 2, Schrödinger demonstrates that the matrices constructed in accordance with the elements of matrix  $F_{jk}$  given by the above-stated equation, with the help of some auxiliary theorems, satisfy the Born-Jordan-Heisenberg laws of motion. More precisely, the Heisenberg-Born-Jordan laws of motion (Born, Heisenberg and Jordan, 1926)—the laws initially derived purely from Matrix Mechanics point of view (Jammer, 1989, 221)—are satisfied by (as Schrödinger characterizes the decisive step in the Introduction) “assigning the auxiliary role to a definite orthogonal system, namely to the system of *proper functions* [Schrödinger’s italics] of that partial differential equation which forms the basis of my wave mechanics” (1926a, 46).

The first indication that Schrödinger believes that the main goal was already achieved in Part 2 with the construction of matrices from eigenfunctions, is his claim at the beginning of Part 3 that he “might reasonably have used the singular” when speaking of Matrix Mechanics and Wave Mechanics. *Yet if we believe that providing a logical proof of the isomorphism between Matrix Mechanics and Wave Mechanics was the central goal of the proof, Part 3 of the text must be at least as essential as Part 2*, as it tries (and ultimately fails) to establish the reciprocal equivalence required by such a goal.

Unlike the pressing issue dealt with in Part 2, the issue addressed in Part 3 is an ‘academic’ (in a pejorative sense of the word) one of logical isomorphism requiring the proof of reciprocal equivalence. Schrödinger states that “the equivalence actually exists, and it also exists conversely.” But he never fully demonstrates this, nor does he make an outstanding effort to do so. Instead, he provides a vague idea of how one might proceed in proving this sort of logical equivalence.<sup>20</sup> More precisely, as Muller (1997a, 56) correctly pointed out, Schrödinger does not prove the bijectivity of the Schrödinger-

---

<sup>19</sup>In other words, the  $H$  turned out to be diagonal with respect to the specified basis (diagonalization of a matrix is a particular orthogonal transformation of the so-called quadratic form, i.e., its rotation).

<sup>20</sup>Muller’s view of what he calls “Schrödinger equivalence” is misleading—Schrödinger ended the proof *vis à vis* eigenvalues in Part 2, contrary to what Muller believes. The “moments problem” of a function issue referred to in Part 3, has to do with the preliminary discussion of the full-fledged logical proof and an attempt to argue for epistemological advantage of Wave Mechanics. Thus, Schrödinger promises “[t]he functions can be constructed from the numerically given matrices.” (p. 58) If so, “the functions do not form, as it were, an *arbitrary* and *special* “fleshly clothing for the bare matrix skeleton, provided to pander to the need of the intuitiveness.” In order to show this, he invokes the totality of the “moments” of a function.

Eckart mapping, necessary for isomorphism.<sup>21</sup>

However, Muller (1997a, 55) misses the bigger picture when he reduces the proof to the narrow model of mathematical equivalence that could be implicit in Part 3 (as well as in his brief discussion of the possibility of Schrödinger's proof being a proof of ontological equivalence in (Muller 1997b)). He leaves out the agreement with Bohr's model of the atom, not realizing that the failure of Part 3 concerning the reciprocal equivalence is not alarming, as it is irrelevant to the central goal. (This is why Muller puzzles over Schrödinger commenting on the subject of bijectivity and reciprocal equivalence in a footnote (Muller, 52).)<sup>22</sup>

In general terms, the constructing of matrices from eigenfunctions in Part 2 becomes meaningful in itself, independently of the reciprocal connection, in light of the final ontological goal of providing a plausible big picture (i.e., Bohr's model). There might be an alternative explanation of the proof's goal<sup>23</sup>, but such an explanation would have to take into account that Schrödinger (and others in their proofs) insisted on the derivation in Part 2 as central. Also, the insistence on the derivation in this direction made sense especially because Matrix Mechanics was not suitable to account for single states.<sup>24</sup>

Moreover, the isomorphism of Matrix Mechanics and Wave Mechanics would have made sense as the *explanans* and as the key, and perhaps, the only goal of the proof, only if a full-blown empirical equivalence was established. Otherwise, given that the ontological and methodological status of Wave Mechanics and Matrix Mechanics was tentative, the more pressing issue of the relation between Matrix Mechanics, Wave Mechanics, and Bohr's model could have been resolved with a "softer" derivation (or, rather, the "construction" of matrices from eigenfunctions)—the kind of derivation devised in Part 2.

The key to the proof, then, is its purported demonstration of the formalisms as essential only through their coherence with Bohr's model. It is not clear why Schrödinger might have insisted on a more demanding and what, at the time, seemed a rather academic and esoteric issue, namely, the logical equivalence of possibly dispensable formalisms. Taken in historical context, the more tangible demonstration was more desirable, especially because establishing Bohr's model as an acceptable "big picture" did not require the logical equivalence (i.e., bi-directional derivation to prove isomorphism). Although ambiguous in his statement of the central goal of the proof, then, Schrödinger likely gave priority to the ontological goal.

A debate with Bohr that immediately resulted in doubts and later led to even more devastating doubts concerning the applicability of Wave Mechanics, took place around the time of writing the proof paper. As expressed in a letter to Wien shortly before the debate, Schrödinger's optimism was diminishing (also reflected in his second

---

<sup>21</sup>Moreover, Part 3 seems to have a further, arguably more important, ontological rather than logical, goal of demonstrating that Wave Mechanics was more than merely an *ad hoc* convenient tool, a sort of a shorthand for the superior Matrix Mechanics, as it was, in Schrödinger's view, perceived by Heisenberg and others (Bitbol, 1996, 68).

<sup>22</sup>It should be noted that despite warning his readers about the danger of reading in Von Neumann's terminology into Schrödinger's text that was developed much later, he does not seem to avoid it entirely himself (Muller, 1997a, 57; Muller 1997b, Section IIIa).

<sup>23</sup>E.g., the equivalence could have been seen as a precursor to the relativistic version of Schrödinger's account, especially because, otherwise, his brief discussion of this issue at the very end of last paragraph seems inserted. Even so, this might not be a competing but rather supplementary goal of the proof.

<sup>24</sup>See quote of Bohr's account on p. 17.

Communication—1926c). This ultimately led him to refocus and to use the soft derivation in Part 2.

Were this not the case, it would be hard to explain the closing passage in the introductory section of the proof, where Schrödinger apparently gets his priorities straight. Although he explicitly emphasizes the construction of matrices from eigenfunctions at the beginning of the paragraph, he only vaguely hints at offering only “a short preliminary sketch” (1926a, 47) of a derivation in the opposite direction as well as the relativistic context of the wave-equation in the last section of the paper. Does this mean that Schrödinger was not keen on the (supposed) main goal of his proof? Or could the passage indicate that he perceived the issue as rather academic?

His characterization of the reversed “construction”<sup>25</sup> would be even more surprising if one believed that Part 3 was the key to the proof. Schrödinger tentatively says, “The following supplement [Schrödinger’s italics] to the proof of equivalence given above is interesting” (Schrödinger 1926a, 58), before going on to discuss the possibility of the construction of Wave Mechanics from Matrix Mechanics and its implications for the epistemological status of Wave Mechanics.<sup>26</sup>

The assertive tone and the insistence on the exclusiveness and superiority of Wave Mechanics over both old quantum theory and Heisenberg’s approach, very explicit in his first Communication (Schrödinger 1926b), and somewhat toned down in the second (Schrödinger 1926c), does not characterize the proof paper. In fact, quite the contrary: the tone of the proof paper is defensive. In Part 3, Schrödinger rather cautiously argues that Wave Mechanics may have the same epistemological significance as Matrix Mechanics does, and, judging by the above-cited passage, treats this portion of the paper as secondary. That Schrödinger set out to, first and foremost, demonstrate the significance of Wave Mechanics (motivated by its agreement with Bohr’s model), a significance which was doubted because of its failure to account for the spectral line intensities, is in keeping with such a tone.

Even if, despite the above-presented indications to the contrary, Schrödinger were at first undecided as to the main goal of the proof, soon after publishing it and his four Communications, he and the quantum physics community embraced it and its limited ontological goal.

Thus, two years after the publication of his seminal work, in his correspondence with others, he continued to discuss the application of the Wave Mechanics and its meaning. Moreover, judging from the following excerpt from Bohr’s 1928 letter to Schrödinger, the key issue was still the nature of the agreement of Wave Mechanics and Matrix Mechanics with Bohr’s (revised) model. Bohr is still concerned with an (implicit) assumption of Matrix Mechanics regarding stationary states as a limitation on the applicability of Wave Mechanics:

In the interpretation of experiments by means of the concept of stationary states, we are indeed always dealing with such properties of an atomic system as dependent on phase relations over a large number of consecutive periods.  
*The definition and applicability of the eigensolutions of the wave equation are*

---

<sup>25</sup> “Construction” is a better word choice than “derivation” in this case, given that the latter might indicate the purely logical nature of the proof.

<sup>26</sup> See footnote 18 for the continuation of Schrödinger’s discussion.

## Why Were Two Theories Deemed Logically Distinct, Yet Equivalent?

---

*of course based on this very circumstance.* (emphasis added; Bohr's letter to Schrödinger (May 23, 1928), in Bohr, 1985, V. 6, 49)

It is also important to compare Schrödinger's effort with similar efforts by others. For instance, in his letter to Jordan (12 April 1926), Pauli talks about "a rather deep connection between the Göttingen mechanics and the Einstein-de Broglie radiation field." (Mehra and Rechenberg, 1982, 656) He thinks he has found "a quite simple and general way [to] construct matrices satisfying the equations of the Göttingen mechanics," a description of the proof's goal which is analogous to the moderate goal of Schrödinger's proof. It is also striking to what extent the use of Bohr's model was critical in constructing the proofs.<sup>27</sup>

### The Moral of the Story

Thus, the 1920s agreement on equivalence appears to be an agreement on a 'myth' only if we leave out the ontological goal of providing a coherent overall model of the atom, and focus solely on the purely formal goal. However, only at a later stage of development was the proof worked out in the terms which Muller's historical and conceptual analysis takes to be central to the 1920s agreement. And although the equivalence of the 1920s was perhaps more provisional than that of the 1930s, it was justified by virtue of its ontological aim.

It is not at all clear, however, that the proof of the equivalence provided by Von Neumann in the 1930s could have settled the issue at the time of the appearance of Schrödinger's proof, given the tentative standing of the formalisms. As Hanson notes, "Von Neumann's theory was a splendid achievement. But it was also a precisely defined mathematical model, based on certain arbitrary, but very clearly stated assumptions concerning quantum theory and its physical interpretation" (Hanson, 1963, 124). In particular, the well-known scattering phenomena could not be formulated in a satisfying way within the limitations of his approach at the time.<sup>28</sup>

In the stage of the development of Quantum Mechanics at which the first set of equivalence proofs was provided, the community of quantum physicists was keen on severe experimental testing of the corpuscular and wave mechanical hypothesis concerning the microphysical processes and their implications. Only after the experiments were judged to have provided satisfying results with respect to the available theoretical accounts (Bohr's model, Matrix Mechanics and Wave Mechanics) did the development of the theory enter the next stage, where an answer to the question of logical equivalence of the two formalisms became significant.

Later commentators understood Schrödinger's proof in the same spirit as Von Neumann (and Muller is right in claiming this) because of the changing tide in quantum physics. The second stage of the quantum revolution had already begun, and physicists concentrated their efforts on the formal aspects of research, grounded on firmly established experimental results. But we should not confuse the subsequent equivocation with the actual understanding of the goals in the 1920s quantum physics community. It is a

---

<sup>27</sup>See (Mehra and Rechenberg, 1982, 657) on Pauli's proof, (D'Abro, 1951, 874) on Dirac's, (Mehra and Rechenberg, 1982, 150) on Heisenberg's and (Scott, 1967, 57) on the proof of Eckart's.

<sup>28</sup>Jammer (1989, 335) also points out some of the difficulties with Von Neumann's approach.

mistake to judge these two stages of the development of quantum theory by a criterion that applies only to the second stage.

Assuming that the proof was justifiably perceived as a breakthrough, what is the moral of the story? How did this affect the understanding of quantum phenomena at the time? What was the importance of the proof, given its domain-specific ontological goal?

Here, Pauli's attitude regarding the results of his own proof are informative. After presenting the relation between Matrix Mechanics and Wave Mechanics in his letter to Jordan, he concluded that, "from the point of view of Quantum Mechanics the contradistinction between 'point' and 'set of waves' fades away in favor of something more general" (Mehra and Rechenberg, 1982, 657). This is strikingly similar to the complementarity view devised by Bohr in response to the same developments.

Also, although at the time there was still a lack of the agreement on the full-fledged empirical equivalence, the proofs demonstrated that the two approaches added up to a coherent account of the atom—at least as far as the known facts went.

In order to appreciate the relevance of this point, it is important to understand that interpretations, formalisms, and the relevant experiments were closely related aspects of the same endeavor. Disentangling them by introducing rigid distinctions might misguide us in our attempts to reconstruct the relevant views and arguments. Both the development of quantum mechanics and its interpretation were closely dependent on the experimental results: the view of the interpretation(s) arising from the theory, and the theory arising from the experiments, is misleading. It is more accurate to say that all three components informed each other.

Thus, the roots of what has become the Copenhagen Interpretation might be found, to a great extent, in the domain-specific ontological equivalence of Matrix Mechanics and Wave Mechanics, not in the manufacturing of consent among physicists and philosophers. If we leave out Bohr's model as the background to the proof(s) and concentrate on the equivalence as a purely mathematico-logical issue, the loose agreement represented by the Copenhagen Interpretation seems to have been enforced. In other words, if we take the background into account, the agreement seems to be a reasonable step forward.

## References

- Beller, M., 1999. *Quantum dialogue*. London and Chicago: The University Chicago Press.
- Bitbol, M., 1995. *E. Schrödinger: The interpretation of quantum mechanics*. Ox Bow Press.
- Bitbol, M., 1996. *Schrödinger's Philosophy of Quantum Mechanics*. Dordrecht: Kluwer.
- Bohr N. (1913). "On the Constitution of Atoms and Molecules," in *Collected Works*, 1984, Vol. 5.
- Bohr, N., 1985. *Collected Works*. North Holland.
- Born, M., Heisenberg, W., and Jordan, P., 1926. "Zur Quantenmechanik II," *Zeitschrift für Physik*, 35, 557–615.

## Why Were Two Theories Deemed Logically Distinct, Yet Equivalent?

---

- Bothe, W. and Geiger, H., 1926. "Ein Weg zur experimentellen Nachprüfung der Theorie von Bohr, Kramers und Slater," *Zeitschrift für Physik*, 26, p. 44.
- Compton, A.H. and Simon, A.W., 1925. "Directed quanta of scattered X-rays," *Physical Review*, 26, pp. 289–299.
- D'Abro, A., 1951. *The Rise of The New Physics*, Dover Publications, New York.
- Dirac, P., 1930. *The Principles of Quantum Mechanics*. Oxford: Clarendon Press.
- Eckart, C., 1926. "Operator Calculus and the Solution of the Equations of Motion of Quantum Dynamics," *Physical Review*, 28, 711–726.
- Gibbins, P., 1987. *Particles and Paradoxes*, Cambridge University Press.
- Hanson, N. R., 1963, *The Concept of the Positron*, Cambridge University Press, Cambridge.
- Heisenberg, W., 1926. "Quantenmechanik," *Die Naturwissenschaften*, 14, 989–995.
- Howard, D., 2004. "Who Invented the 'Copenhagen Interpretation?' A Study in Mythology," *Philosophy of Science*, Vol. 71, No. 5, pp. 669–683
- Hund, F., 1974. *The History of Quantum Theory*. London: Harrap.
- Jammer, M., 1989. *Conceptual Development of Quantum Mechanics*, American Institute of Physics.
- Mehra, J. and Rechenberg, H., 1982. *The Historical Development of Quantum Mechanics*. New York: Springer Verlag.
- Muller, F. A., 1997a. "The Equivalence Myth of Quantum Mechanics—Part I," *Studies in History and Philosophy of Science Part B: Studies in History and Philosophy of Modern Physics*, Vol. 28, Issue 1, pp. 35–61
- Muller, F. A., 1997b. "The Equivalence Myth of Quantum Mechanics—Part II," *Studies in History and Philosophy of Science Part B: Studies in History and Philosophy of Modern Physics*, Vol. 28, Issue 2, pp. 219–247
- Neumann, J. von, 1932. *Mathematical Foundations of Quantum Mechanics*. Translated by R. T. Beyer (Princeton: Princeton University Press, 1935)
- Pauli, W., 1926. "Über die Wasserstoffspektrum Vom Standpunkt der Nuen Quantenmechanik," Waerden, B. L., Van der, ed., 1967., *Sources of Quantum Mechanics*, Amsterdam: North-Holland, pp. 387–416
- Perovic, S., 2006. "Schrödinger's Interpretation of Quantum Mechanics and the Relevance of Bohr's Experimental Critique," *Studies in History and Philosophy of Science Part B: Studies in History and Philosophy of Modern Physics*, Vol. 37/2, pp. 275–297.
- Ramsauer, C., 1921. "Über der wirkungsquerschnitt der gasmoleküle gegenüber langsamen elektronen," *Annalen der Physik*, 72, 345–352.



- Schrödinger, E., 1926a. "On the Relation between the Quantum Mechanics of Heisenberg, Born, and Jordan, and that of Schrödinger," *Collected Papers on Wave Mechanics*, New York: Chelsea Publishing Company, 45–61. Originally in *Annalen der Physik (4)*, Vol. 79.
- Schrödinger, E., 1926b. "Quantisation as a Problem of Proper Values—I," *Collected Papers on Wave Mechanics*, 1–12. Originally in *Annalen der Physik (4)*, Vol. 79.
- Schrödinger, E. 1926c. "Quantisation as a Problem of Proper Values—II," *Collected Papers on Wave Mechanics*, 13–40. Originally in *Annalen der Physik (4)*. Vol. 79.
- Scott, W. T., 1967. *Erwin Schrödinger: An Introduction to His Writings*. University of Massachusetts Press.
- Stuewer, R., 1975. *The Compton Effect*, New York: Science History Publications.
- Suppes, P., 1957. *Studies in the Foundations of Quantum Mechanics*. East Lansing, MI: Philosophy of Science Association.
- Suppes, P., 1960. "A comparison and the Meaning and Use of Models in Mathematics and Empirical Sciences," *Synthese*, 12, pp. 287–301
- Van der Waerden, B. L. 1973. "From matrix mechanics and wave mechanics to unified quantum mechanics," Mehra, J., ed., *The Physicist's Conception of Nature*, D. Riedel Publishing Company, Dordrecht-Holland, Boston-USA

# 12 Planck and de Broglie in the Thomson Family

JAUME NAVARRO

## Introduction

The 1927 Solvay Conference is usually regarded as one of the central moments in the history of the development and acceptance of the new quantum physics. In that meeting, the latest developments in both wave and matrix mechanics were publicly discussed by the main characters of this drama. In the years after the Great War, German and Austrian scientists had been banned from international meetings, a fact that eventually helped Bohr's institute, in neutral Copenhagen, to become the focal point of international discussions on the new physics. The fifth Solvay conference was the first to waive the boycott that had been in place in the two previous councils (the ones of 1921 and 1924), and thus it became a unique opportunity to gather all the major actors of quantum physics under the same roof.<sup>1</sup>

Only a month before the Solvay meeting in Brussels, a huge international event gathered hundreds of physicists in Como, Italy, in a celebration of Alessandro Volta and Italian science. There, Niels Bohr was invited to open a discussion on quantum physics by giving an overview of the latest developments in the new science. Werner Heisenberg, Wolfgang Pauli, Enrico Fermi and Max Born were among the participants in the discussion. But others were missing: Albert Einstein and Erwin Schrödinger were absent, probably for political reasons. Louis de Broglie, whose contribution had been so crucial in the last three years, was also absent in Como.

At one point of his speech in Como, Bohr signalled that “recent experience, above all the discovery of the selective reflection of electrons from metal crystals, requires the use of the wave theoretical superposition principle in accordance with the original ideas of L. de Broglie”,<sup>2</sup> better known as the principle of wave-particle duality. Bohr was referring here to the experiments reported by American physicists Clinton J. Davisson and Lester H. Germer. Oblivious to the intricacies of the new quantum physics, Davisson and Germer were working on the scattering of electrons on metallic surfaces, as part of their research in the industrial Bell Laboratories. The anomalous results they had been obtaining since 1923 only made sense after a young student of Max Born in Göttingen, Walter M. Elsasser, suggested in 1925 that they could be interpreted in terms of electron diffraction. In early 1927, Davisson and Germer reported final evidence of the diffraction of electrons in their scattering by metal plates, thus proving the wave behaviour of the

<sup>1</sup>See Pierre Marage and Gregoire Wallenbron, eds., *The Solvay Conferences and the Birth of Modern Physics* (Basel; Boston, Mass : Birkhäuser Verlag, 1999).

<sup>2</sup>Niels Bohr, “The quantum postulate and the recent development of atomic theory”, in *Atti del Congresso Internazionale dei Fisici*, vol. 2, (Bologna : N. Zanichelli, 1928), 568.

electrons.

When, a month later, Louis de Broglie presented his paper at the Solvay Conference, he made a serious effort to update on the experimental results that might support his theory of wave-particle duality. Together with the experiments of Davisson and Germer, to which he devoted thorough attention, he also mentioned the latest observations of George Paget Thomson and his student, Alexander Reid, only recently published as a preliminary note in *Nature*. In that note, Thomson and Reid published a photograph obtained after “a beam of homogeneous cathode rays is sent through a thin celluloid film”, in which “the central spot formed by the undeflected rays is surrounded by rings, recalling in appearance the haloes formed by mist round the sun”.<sup>3</sup> In de Broglie’s words, “these observations are very interesting and they confirm, although only roughly, the new conceptions”.<sup>4</sup>

Ten years later, in 1937, Davisson and Thomson shared the Nobel Prize for their experimental confirmation of the undulatory nature of the electrons and, therefore, the principle of duality wave-particle put forward by de Broglie. Their experimental paths were largely distinct, and this helped to have two independent confirmations of the radical principle of wave-particle duality. Historical analysis on the work of Davisson and Germer was done by historian of science Arturo Russo more than 25 years ago.<sup>5</sup> On the contrary, the work of G. P. Thomson has never received sufficient attention by historians of quantum physics. This neglect can be partly due to the fact that British physicists played but a minor role in the theoretical developments of quantum physics and, therefore, are of little significance in a whiggish history of science. However, the current project in the analysis of the early developments of quantum physics opens the door to the study of what one might be tempted to call ‘the losers’, i.e., those who didn’t fully accept the radical changes of the new physics.

In this paper I want to discuss the intellectual setting in which G.P. Thomson developed his early career, a career that was boosted by the experiments of 1927. As I shall argue, the influence of his father, Sir Joseph John Thomson, proved to be a crucial factor in the way G.P. received quantum physics. As most Victorian scientists, J.J. was not prepared to accept the quantum of action as a metaphysical principle: his world was a world of ether and, therefore, essentially continuous. Any discreteness in physical theories was only phenomenological. This worldview was preserved within the Thomson family and this explains G.P.’s difficulties in understanding the relevance of the new physics. Far from becoming an *experimentum crucis*, electron diffraction was a proof, to J.J.’s eyes, of the correctness of his worldview of ether. Only partly did G.P. manage to cut the umbilical cord that had kept him tied to his father’s metaphysics in the beginning of his career.

---

<sup>3</sup>George P. Thomson and Andrew Reid, “Diffraction of Cathode Rays by a Thin Film”, *Nature* 119 (1927), 890.

<sup>4</sup>Louis de Broglie, “La Nouvelle Dynamique des Quanta”, in *Electrons et photons. Rapports et discussions du cinquieme conseil de physique tenu a Bruxelles du 24 au 29 Octobre 1927 sous les auspices de l’Institut International de Physique Solvay* (Paris, 1928), 130.

<sup>5</sup>See Arturo Russo “Fundamental research at Bell Laboratories: The discovery of electron diffraction” *Historical Studies in the Physical Sciences* 12 (1981), 117–160.

## J.J. and the quantum of light (c. 1925)

J.J. Thomson's world was a world of ether. Ever since his work for the 1881 Adams Prize, Thomson had attempted to understand matter as an epiphenomenon of the ether. First, it was the vortex-ring theory, which had its origins in Helmholtz and Kelvin;<sup>6</sup> and then, around 1891, he shifted to the notion of Faraday tubes of force, a theoretical tool he kept, in different formats, all his life.<sup>7</sup> Faraday tubes were bundles of lines of force in the ether, acting as the channels of energy between charged bodies. In 1891 he defined them in the following way:

“...the electric field is full of tubes of electrostatic induction, that these are all of the same strength, and that this strength is such that when a tube falls on a conductor it corresponds to a negative charge on the conductor equal in amount to the charge which in electrolysis we find associated with an atom of a univalent element. These tubes must either form closed circuits, or they must end on atoms, any unclosed tube being a tube connecting two atoms”.<sup>8</sup>

Always eager to promote mental images in the development of physical theories, Thomson rejected the interpretation of Maxwell's theories only in terms of dimensional equations.<sup>9</sup> Eventually, however, the tubes of force ceased to be only a mental image and became a physical reality. In 1925, he explained: “I suppose that these lines are not merely geometrical figments, but that they, or rather the groups of them forming tubes of force (...), are physical realities, and that the energy in the electric field is bound up with these tubes”.<sup>10</sup>

Since the tubes of force were real physical entities, and not merely ideal devices, this meant that there should be an actual physical limit to their divisibility.<sup>11</sup> This idea opened the door to a quantification of energy and charge within the framework of a continuous ether. Continuity and discreteness were, in this way, aspects of nature which were not mutually exclusive.

The tubes of force were instrumental in the experiments that led J.J. to the discovery of the electron; and he retrieved them in the early 1900s to give a particular account that would explain the structure of light. Ever since the discovery of X-rays, the old problem of explaining light in terms of either waves or particles gained particular momentum. J.J. was no alien to this problem. As an expert on the interaction between electricity and matter in discharge tubes, Thomson became increasingly aware of the discrete behaviour

<sup>6</sup>See Helge Kragh, “The Vortex Atom: A Victorian Theory of Everything” *Centaurus* 44 (2002), 32–126; and Jaume Navarro, “J.J. Thomson on the nature of matter: corpuscles and the continuum” *Centaurus* 47 (2005), 259–282.

<sup>7</sup>For the reasons why he shifted from vortex rings to Faraday tubes, see Isobel Falconer, “Corpuscles, Electrons and Cathode Rays: J.J. Thomson and the ‘Discovery of the Electron’” *British Journal for the History of Science* 20 (1987), 241–276.

<sup>8</sup>Joseph J. Thomson, “On the Illustration of the Properties of the Electric Field by Means of Tubes of Electrostatic Induction” *Philosophical Magazine* 31 (1891), 149–171, 150.

<sup>9</sup>See David Topper, “‘To reason by means of images’: J.J. Thomson and the mechanical picture of Nature” *Annals of Science* 37 (1980), 31–57.

<sup>10</sup>Joseph J. Thomson, *The Structure of Light* (Cambridge: Cambridge University Press, 1925), 20.

<sup>11</sup>Joseph J. Thomson, *Notes on recent researches in electricity and magnetism: intended as a sequel to Professor Clerk-Maxwell's Treatise on electricity and magnetism* (Oxford: The Clarendon press, 1893), 3.

of both matter and light. Being one of the first researchers in Britain to use X-rays in his laboratory work (an innovation that was, by the way, instrumental to his discovery of the corpuscle-electron), he soon engaged in efforts to explain the apparently dual nature of Röntgen rays and, by extension, of any light wave. The properties of the photoeffect confirmed Thomson in his intuition that there was a certain discreteness in the wave front of electromagnetic waves.

His idea that the tubes of force, the carriers of electromagnetic energy, were both continuous and discrete led him to suggest a theory of light in which the wave front was discontinuous:

“This view of light as due to the tremors in tightly stretched Faraday tubes raises a question which I have not seen noticed. The Faraday tubes stretching through the ether cannot be regarded as entirely filling it. They are rather to be looked upon as discrete threads embedded in a continuous ether, giving to the latter a fibrous structure; but if this is the case, then on the view we have taken of a wave of light the wave itself must have a structure, and the front of the wave, instead of being, as it were, uniformly illuminated, will be represented by a series of bright specks on a dark ground, the bright specks corresponding to the places where the Faraday tubes cut the wave front”.<sup>12</sup>

This theory was, however, never developed beyond the realm of ideas and suggestions. There was never a complete mathematical development that would validate the theory or, otherwise, point at its limitations.

It was not until 1909 that Thomson publicly gave his opinion on what he called the “light-quantum hypothesis” of Planck. It was the beginning of his long controversy with the increasingly popular quantum theory, a controversy in which “Thomson’s basic position was that energy itself has no coherence, or inherent structure, but rather that the carriers of the energy—Faraday tubes, electrons, etc.—are the permanent, indivisible entities”.<sup>13</sup> This was, however, already an advanced mentality compared to most British physicists in the first decade of the 20th century. J.J. was, at least, ready to accept a certain discontinuity in the electromagnetic waves and the ether, as his early theory on the structure of light shows.

J.J. could not accept Planck’s theory basically for two reasons. First, because the way he read Planck (closer to Einstein’s interpretation of the quantum) involved a quantification of energy itself. Thomson was ready to accept a quantification of the carriers of energy (as he had accepted a quantification of the carriers of charge), but nothing beyond this point. And second, because Planck’s theory, while explaining the discrete phenomena in radiation was not able to explain the wave characteristics of light such as diffraction. Not that his models could, but preserving the ether was a way to keep the door open to both discrete and undulatory characteristics.

The following quotation helps us to illustrate the grounds of his opposition to Planck’s hypothesis while, at the same time, accepting the possibility of a certain quantification:

“Again, if all the atoms were made of vortices of the same ‘strength’, we should find that certain mechanical quantities would all be integral multiples

---

<sup>12</sup>Joseph J. Thomson, *Electricity and Matter* (London: Archibald Constable & Co, 1906), 62–63.

<sup>13</sup>Russell McCormach, “J.J. Thomson and the Structure of Light” *British Journal for the History of Science* 3 (1967), 362–387, 375.

of a definite unit, i.e. these dynamical quantities, though not matter, would resemble matter in having an atomic constitution, being built of separate indivisible units. The quantity known as ‘circulation’ is proportional to its moment of momentum, and we see that in a theory of this kind the moment of momentum of particles describing circular orbits would always be an integral multiple of a definite unit. We see from this example that when we have a structure as fine as that associated with atoms, we may find dynamical quantities such as moment of momentum, or it may be kinetic energy, assuming the atomic quality and increasing or decreasing discontinuously by finite jumps. In one form of a theory which has rendered great service to physical science—I mean Planck’s theory of the ‘quantum’—the changes from radiant to kinetic energy are supposed to occur not continuously, but by definite steps, as would inevitably be the case if the energy were atomic in structure. I have introduced this illustration from the vortex atom theory of matter, for the purpose of showing that when we have a structure as fine as that of atoms we may, without any alteration in the laws of dynamics, get discontinuities in various dynamical quantities, which will give them the atomic quality. In some cases it may be that the most important effect of the fineness of the atomic quality in some dynamical quantity such as the kinetic energy. If then we postulate the existence of this propriety for the energy, it may serve as the equivalent of a detailed consideration of this structure itself. Thus, for many purposes (...) Planck’s quantum theory serves as the equivalent of a knowledge of the structure of the atom”.<sup>14</sup>

In 1910, J.J. introduced a new modification in his theory of light which is relevant for the purposes of this paper. He suggested that every single electron was the origin of only one Faraday tube of force and, therefore, each of the electrons exercised its influence only in one direction.<sup>15</sup> This enabled him to visualize better the concentration of energy in apparently corpuscular form: the impulse produced by a rapid displacement of an electron would be represented as a kink in the Faraday tube, a kink that would not spread but only travel in the direction of the tube.<sup>16</sup> In this way he had no need to postulate a quantum of light, since the apparent quantification was only a consequence of the way energy spread within a physical tube of force.

With these elements in mind, and with a growing interest to disprove Planck’s notion that energy was essentially discrete, J.J. kept presenting different modifications to his theory of light. The one that interests me for the argument of this paper is a mechanism he presented in 1924 to account for the apparent discrete behaviour of light. Based, yet again, on the Faraday tubes of force, J.J. suggested that,

“on this view the mutual potential energy of an electron  $E$  and a positive charge  $P$  is located in the tube of force stretching between  $E$  and  $P$ . If the electron falls from  $E$  to  $E'$  this potential energy is diminished by the energy

<sup>14</sup>Joseph J. Thomson, *The Atomic Theory. The Romanes Lecture* (Oxford: The University Press, 1914), 26–27.

<sup>15</sup>Joseph J. Thomson, “On a Theory of the Structure of the Electric Field and its Application to Röntgen Radiation and to Light” *Philosophical Magazine* 20 (1910), 301–313.

<sup>16</sup>See Bruce R. Wheaton, *The Tiger and the Shark: Empirical roots of wave-particle dualism* (Cambridge: Cambridge University Press, 1983), 140–142 for an analysis of this theory.

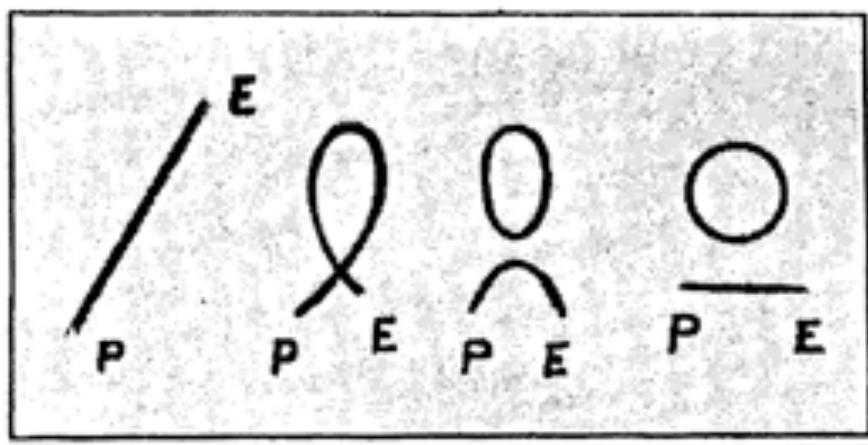


Figure 12.1: Bending of the Faraday tube

in the portion  $EE'$  of this tube of force; for the energy in this portion to get free and travel out as light, the piece  $EE'$  of the tube must get into a state where it can travel freely with the velocity of light and not be associated with a charge of electricity whether positive or negative”.<sup>17</sup>

As illustrated in Fig. 12.1, when an electron jumped from a certain energy state to a lower one, the Faraday tube would bend. If the bent was big enough as to create a closed loop of tube of force, this would disassemble from the main body of the tube, giving rise to a “closed ring, which rapidly becomes circular and travels with the velocity of light. (...) The energy of this ring, (...) remains constant as long as the ring is unbroken”.<sup>18</sup> That would be, in the terminology of quantum physics, the quantum of light. Analogously, the reverse process would explain the absorption of light and the jumping of the electron to a level of higher energy.

“Thus we see that the death of a ring means either the birth of a high-speed electron or the emission of a unit of characteristic radiation. (...) The rings are the centres in which the energy from light to matter involves the destruction of these rings; thus the amount of energy transferred from a beam of monochromatic light or homogenous Röntgen radiation must be an integral multiple of a unit”.<sup>19</sup>

This unit was, of course, Planck’s constant.

A last aspect to point at is the way J.J. was trying not only to account for discrete phenomena but also for the continuous aspects of light, especially diffraction. The process of creation and emission of a ring of Faraday tube is such that before and after the emission of the ring the ether around the vibrating electron is set in motion. The ring itself, when liberated, is also vibrating. This gives us the picture of a ring which “will be

<sup>17</sup>Joseph J. Thomson, “A suggestion as to the Structure of Light” *Philosophical Magazine* 48 (1924), 737–746.

<sup>18</sup>*Ibid.*, 738.

<sup>19</sup>*Ibid.*, 739.

the centre of a system of electrical waves of the normal type, and predominant among these are those which have the same periodicity as the vibrations of the ring”.<sup>20</sup> If the ring is assimilated to a unity of light, we find that this is accompanied by an extended wave. Thus, Thomson gets a picture in which discrete entities go hand in hand with undulatory characteristics, by which he aimed at an understanding of the dual nature of light and radiation.

The occurrence of diffraction in the passage of light through a slit would be explained in the following terms:

“If the waves surrounding the ring fall on a narrow slit in a metal plate parallel to the plane of the ring, the electric and magnetic forces in the parts of the wave in the slit are much greater than they were before the wave reached the slit. The directions of these forces change as well as their intensities, so that the Poynting vector, i.e. the direction of the flow of energy, will change in direction from place to place in the neighbourhood of the slit. Thus the flow of energy gets diverted when the wave passes through the slit; it is no longer always in one direction, but spreads out fanwise after leaving the slit”.<sup>21</sup>

In a famous statement in 1925, J.J. referred to the tension between discrete and undulatory conceptions of light as the battle between a tiger and a shark: “the position is thus that all optical effects point to the undulatory theory, all the electrical ones to something like the corpuscular theory; the contest is something like one between a tiger and a shark, each is supreme in its own element but helpless in that of the other”.<sup>22</sup> His mental model was a step towards solving this entanglement; and it was a model that predisposed him favourably towards de Broglie’s ideas. Furthermore, his theory of light was, in J.J.’s mind, more powerful than the, by then, “universally accepted” law of Planck. The latter was giving a good account of discrete phenomena in light, but “it is quite foreign to the undulatory theory which postulates a continuous and not an atomic distribution of energy”.<sup>23</sup> Thus, J.J. always considered Planck’s law as an incomplete theory that was solving the corpuscular aspects of light without explaining its undulatory properties.

### G.P. and de Broglie’s Principle

George Paget Thomson belongs to that special brand of British physicists whose entire life evolves around the University of Cambridge. Born in that university town in 1892, G.P. was the first and only son of J.J. who subtly led him into a career in physics. He was prepared by private coaching even before his enrolment in the university and, as a result, he was able to sit for both the Mathematical Tripos and the Natural Sciences Tripos in the three customary years that people took for only one degree. This gave him a special training in which both theoretical and experimental aspects of physics

---

<sup>20</sup> *Ibid.*, 740.

<sup>21</sup> *Ibid.*, 741.

<sup>22</sup> J. J. Thomson, *op. cit.* (10), 15.

<sup>23</sup> *Ibid.*



were present. Nevertheless, the particular training G.P. received in pre-World War I Cambridge was totally oblivious to the new developments in quantum theory.

In Cambridge, quantum physics and relativity were not formally taught until after the Great War, and even then only in the form of ‘special courses’: Charles Galton Darwin gave a course on spectra and quantum physics, and Arthur Eddington a course on relativity. Darwin was, together with Ralph Fowler, one of the first to introduce the new quantum physics in Cambridge.<sup>24</sup> A good life-long friend of G.P., Darwin became very critical of “the deficiencies of the syllabus [in Cambridge] which was disconnected from the subjects then coming into importance”.<sup>25</sup> After graduating in Cambridge, Darwin moved to Manchester, where he met Niels Bohr in the crucial years of the development of his atomic model. This was his first real contact with the new physics and, after the war, when he returned to Cambridge as fellow of Christ’s College, he was ready to embrace and work on quantum physics. Fowler’s engagement with the new science was more independent than Darwin’s. It was during the war, after being wounded in Gallipoli, that Fowler could study quantum physics from German scientific journals. Both Darwin and Fowler were Cambridge contemporaries and good friends of G.P., and he relied on them to get introduced into the new quantum physics in the late 1920s. During his formative years, quantum principles were rarely mentioned at home or in the university, and when they were, it was with high doses of contempt.

A faithful and devoted son of his father, G.P. relied on the advice of J.J. who became his mentor and supervisor in his first research work at the Cavendish. This is the reason why G.P. started his career as a researcher in the Cavendish laboratory on a project to study the nature and behaviour of positive rays. This project would eventually lead J.J.’s other assistant, F.W. Aston, to the manufacturing of the mass spectrometer and the discovery of isotopes. For J.J., however, as much as for G.P., this project had a different interest: first, the study of positive electricity emulating J.J.’s early work on cathode rays, and later, in the 1920s, as an instrument for chemical analysis. And the latter was the project that G.P. took with him to Aberdeen when he was appointed Professor of Natural Philosophy, in 1923.

While he was working with valves, sealing glass tubes, and pursuing the fine tuning of the vacuum pump in Aberdeen, G.P. was not oblivious to the theoretical developments of physics. His very good friends from the days of Cambridge—Darwin, Fowler and Bragg—would keep him up-to-date on their respective researches. It thus comes as no surprise that G.P. was well aware of de Broglie’s principle, recently translated into English with the backing of Fowler.<sup>26</sup> In that paper, de Broglie was presenting the results of his recent PhD dissertation, from which he was “inclined to admit that any moving body may be accompanied by a wave and that it is impossible to disjoin motion of body and propagation of wave”.<sup>27</sup> This is what soon came to be understood as the

---

<sup>24</sup>See the *Cambridge University Reporter*. In 1919 Darwin offered a course on ‘Quantum Theory and Origin of Spectra’. This course changed to ‘Recent Developments on Spectrum Theory’ the following year, and a joint course on isotopes with Aston in 1921. In 1922 Fowler gave his first special course on ‘The Theory of Quanta’.

<sup>25</sup>George P. Thomson, *J.J. Thomson and the Cavendish Laboratory in his Day* (London and Edinburgh: Thomas Nelson and Sons, 1964), 70.

<sup>26</sup>Louis de Broglie, “A tentative theory of Light quanta” *Philosophical Magazine* 47 (1924), 446–458. This paper was communicated by Ralph Fowler.

<sup>27</sup>*Ibid.*, 450.

principle of duality wave-particle, and which Schrödinger eventually turned into a full formulation of a wave quantum mechanics.<sup>28</sup>

De Broglie's English paper was entitled "A Tentative Theory of Light Quanta", a title which had very strong resonances in the Thomson family. As seen above, the nature of light and the other radiations had been a topic of heated debates for the past twenty years; a debate in which J.J. had been one of the main actors. This paper by de Broglie was an attempt to design a new theory of light, as much as J.J.'s 1924 paper was. Both were published in the same year and G.P. tried to unite them in a paper in the *Philosophical Magazine*. In retrospect, G.P. would regret publishing this paper, calling it "an example of a thoroughly bad theoretical paper",<sup>29</sup> even though it was proof, in his reconstructions of history, that he had paid attention to de Broglie's theory as soon as it was published in the British milieu: "I think in retrospect I was in advance of my time, I think I paid more attention to de Broglie than probably anybody else in this country on the whole. Some people thought it was just nonsense".<sup>30</sup>

The point to stress here is that G.P. knew of de Broglie's theory as a theory of light and electronic orbits, not as a theory of electron diffraction.<sup>31</sup> As we shall see, the idea of electron diffraction as an experimental application of de Broglie's theory came to him only some time in the summer of 1926, not in 1924. The title of his 1925 paper is "A Physical Interpretation of Bohr's Stationary States", and in it he tries to dismiss de Broglie's radical hypothesis as unnecessary. If the trajectories of electrons were understood in terms of waves as much as of particles, only those orbits in which the path is a multiple of the wavelength can be stable orbits around the nucleus, a suggestion that was totally in tune with Bohr's quantification. G.P.'s suggestion was that these stationary states could be equally achieved following his father's 1924 atomic model explained above. If proton and electron were united by a Faraday tube of force, "it will thus be able to transmit waves, and the condition that will be taken as determining the possible states is that the vibrations in this tube shall be in tune with the period of the orbit".<sup>32</sup> In this manner, G.P. Thomson was doing away with the main characteristic of de Broglie's hypothesis—the fact that electrons were actually waves—by ascribing the wave motion to the tube of force *outside* the electron.

---

<sup>28</sup>For this process, see Varadaraja V. Raman and Paul Forman, "Why was it Schrödinger who developed de Broglie's ideas?" *Historical Studies in the Physical Sciences* 1 (1969), 291–314.

<sup>29</sup>George P. Thomson, "Early Work in Electron Diffraction" *American Journal of Physics* 29 (1961), 821–825, 821.

<sup>30</sup>Oral interview with George P. Thomson, *Archive for the History of Quantum Physics*, Tape T2, side 2, 8.

<sup>31</sup>In his reconstruction of the events, G.P. presented a different version of the facts. G.P. Thomson, *op. cit.*, (29), 821: "At that time we were all thinking of the possible ways of reconciling the apparently irreconcilable. One of these ways was supposing light to be perhaps particles after all, but particles which somehow masqueraded as waves; but no one could give any clear idea as to why this was done. The first suggestion I ever heard which did not stress most of all the behaviour of the radiation came from the younger Bragg, Sir Lawrence Bragg, who once said to me that he thought the electron was not so simple as it looked, but never followed up this idea. However, it made a considerable impression on me, and it pre-disposed me to appreciate de Broglie's first paper in the *Philosophical Magazine* of 1924".

<sup>32</sup>George P. Thomson, "A physical interpretation of Bohr's stationary states" *Philosophical Magazine* 1 (1925), 163–164, 163.

## G.P.'s experiments on electron diffraction

“By 1926 I was feeling depressed by having failed to produce anything of real note. In fact, positive rays, as distinct from the study of isotopes, were nearly worked out, at least for the time”.<sup>33</sup> Looking at his laboratory notebooks, however, no hint of G.P.'s disappointment is evident: in the first half of the year he keeps accumulating data and changing the experimental conditions in his work on positive rays. The last entry before the summer break is from June 23rd, in which he is testing the scattering of positive rays in Argon; the next entry, on August 23rd, clearly signals a shift of research project: “Alteration to apparatus. A slip of gold leaf mounted on brass carrier + partly covering aperture in camera”.<sup>34</sup> His quest for electron diffraction had started.

The different autobiographical notes by G.P. on the events leading up to his measurement of electron diffraction are a bit hazy. They all coincide, however, as does all other evidence, in assigning a central role to the month of August 1926, both in Oxford and in Cambridge. From the 4th to the 11th the British Association for the Advancement of Science held its annual meeting in Oxford; and it became the forum in which many British and American physicists learnt about the latest developments in wave quantum mechanics. During the spring that year Erwin Schrödinger, based on de Broglie's ideas, had reinterpreted wave mechanics from a quantum perspective. Max Born, present at the meeting, explained these developments to the participants, and the topic became one of the highlights in the informal discussions in the meeting.<sup>35</sup>

Straight after the Oxford meeting G.P. stopped over in Cambridge, where he could continue discussions on electron diffraction. Actually, in the Cavendish he must have met with Charles D. Ellis, who had, as early as 1924, unsuccessfully tried to convince Rutherford to allow him to look for electron diffraction in the Cavendish.<sup>36</sup> The case is that be it in conversations in Oxford or in Cambridge, G.P. saw—or was led to understand—that his experimental device in Aberdeen was all that was needed to try electron diffraction through solids and that he was in the best of conditions to give it a try. And that's what he did, first with his research student Andrew Reid, and then, after the unfortunate death of the latter in a motorcycle accident, on his own. The first tentative results were published in a note in *Nature* in June 1927,<sup>37</sup> and this was followed by a full account of his work in several articles later that year and the following one.<sup>38</sup>

<sup>33</sup>George P. Thomson Archives, Trinity College, Cambridge, A6, 7.

<sup>34</sup>*Ibid.*, C24, 13.

<sup>35</sup>Born's paper had a strong impact on many of the present, but especially on the American physicist working at the Bell laboratories, Clinton J. Davisson, when he heard that the anomalous results he had been obtaining in experiments on electron dispersion with his colleague Lester H. Germer might be signs of electron diffraction. That branch of the story, which was studied in detail by historian of science Arturo Russo, ends with the confirmation of electron diffraction in the Bell laboratories and the sharing of the Nobel Prize with G.P. Thomson for their experimental proof of de Broglie's principle. Born also mentioned the experiments of the young German physicist, Walter M. Elsasser, who had unsuccessfully tried to detect diffraction patterns in the passage of an electron beam through a metallic film. See Arturo Russo, *op. cit.* (5).

<sup>36</sup>*Ibid.*, 141.

<sup>37</sup>George P. Thomson and Andrew Reid, “Diffraction of Cathode Rays by a Thins Film” *Nature* 119 (1927), 890.

<sup>38</sup>George P. Thomson, “The Diffraction of Cathode Rays by Thin Films of Platinum” *Nature* 120 (1927), 802; “Experiments on the Diffraction of Cathode Rays” *Proceedings of the Royal Society* 117 (1928), 600–609; “Experiments on the Diffraction of Cathode Rays. II” *Proceedings of the Royal Society* 119

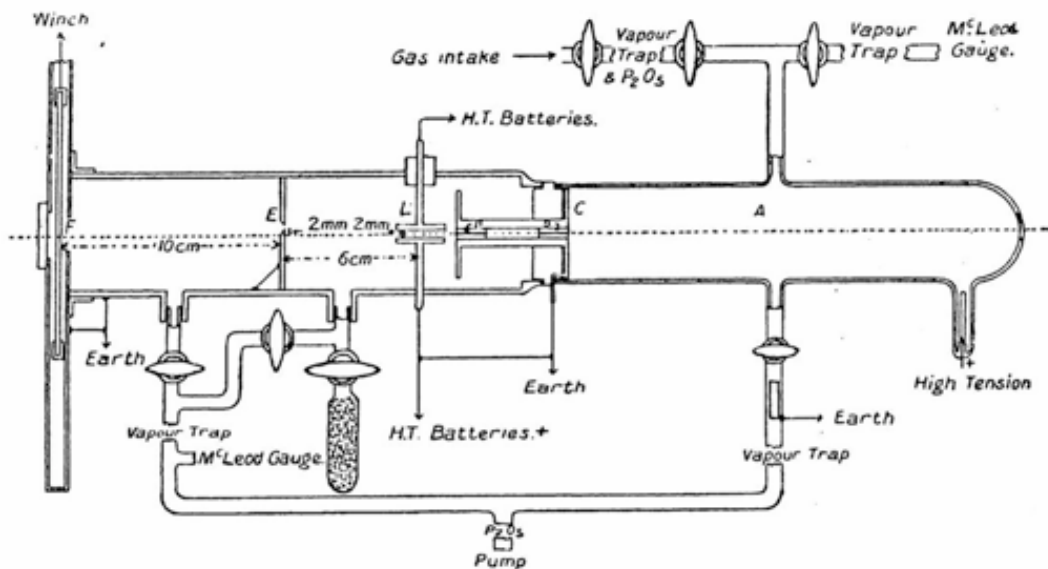


Figure 12.2: Experimental Arrangement

A quick comparison between the experimental arrangement he had so far used for his experiments on positive rays (Fig. 12.2) with the one he used in his work of 1926–1927 clearly shows that few changes were needed for the new measurements. His original display provided positive rays using a cathode rays tube; and now, the same tube could be the source of a beam of electrons. The “apparatus for studying the scattering of positive rays (...) could be used for this experiment with little more change than reversing the current in the gaseous discharge which formed the rays”.<sup>39</sup> The rest of the arrangement only varied in the fact that instead of scattering the positive rays in a gas, he would attempt their diffractive dispersion through a thin metallic plate. The latter was, in a way, the only real experimental change, one in which he depended on the good skills of his assistant C.G. Frazer, who succeeded in obtaining the extremely thin metallic films that were needed.

The aim of this paper is not to give a detailed account of G.P.’s work in the period 1926–1928. But one element needs to be highlighted: the close connection between his experiments and the long tradition in research on X-ray diffraction, to which G.P. was certainly no stranger. After the discovery of X-ray diffraction by Planck’s protégé Max von Laue in Munich in 1912, G.P.’s life-long friend Lawrence Bragg had modified his father’s research project on X-rays and understood that X-ray diffraction could be used as a tool to determine the crystalline structure of metals. This other father-son story culminated in the shared Nobel Prize that both Braggs received in 1915 and, most importantly, consolidated the emergence of the new science of X-ray crystallography in Britain. G.P. certainly followed closely these developments due to his friendship with

(1928), 651–663; “Experiments on the Diffraction of Cathode Rays. III” *Proceedings of the Royal Society* 125 (1929), 352–370.

39

the young Bragg with whom he spent summer holidays in G.P.'s boat, the *Fortuna*.<sup>40</sup> His other life-long friend, C. G. Darwin, was responsible for the formulation of the most successful theory of X-ray diffraction between 1913 and 1922.<sup>41</sup>

The parallelism between G.P.'s experiments and X-ray diffraction was almost complete, since the order of energy of the waves de Broglie was talking about was the same as that of hard X-rays. The only real difference between X-rays and the waves of cathode rays was that the latter could be deflected with electric and magnetic fields due to their electric charge, a difference that proved essential in order to make sure that the diffracted patterns were not due to secondary X-rays but to the cathode rays themselves.<sup>42</sup> Again, this was a feature that the experimental arrangement for G.P.'s project on positive rays already included: like the experiment that had led to the hypothesis of the corpuscle in 1897, the Thomsons' study on positive rays involved their deflection by electric and magnetic fields in the glass tube.

The pictures G.P. obtained were powerful enough to convince his audience (Fig. 12.3). The circular halos were widely recognised as the Hull-Debye-Scherrer patterns of diffraction, already known for X-ray diffraction. Therefore, if those pictures were really obtained from dispersed cathode rays, there was no other way out but to accept that the electrons behaved like waves: "The detailed agreement shown in these experiments with the de Broglie theory must, I think, be regarded as strong evidence in its favour".<sup>43</sup>

If the period between the summer of 1926 and the spring of 1928 required only a few changes in the experimental culture of G.P. Thomson, it did however involve a radical change in his conceptual framework. Distancing himself from his classical tradition, he was suddenly coming to terms with the fact that, as he said in his November 1927 paper, his experiments involved "accepting the view that ordinary Newtonian mechanics (including the relativity modifications) are only a first approximation to the truth, bearing the same relation to the complete theory that geometrical optics does to the wave theory".<sup>44</sup> This statement strongly suggests a connection with Niels Bohr's correspondence principle, formulated in 1923, by which it is assumed that classical physics is the limit of quantum physics for large quantum numbers. If that is so, that would mean a first abandonment of the classical mechanics he had thus far been immersed in, and one

---

<sup>40</sup>See Graeme K. Hunter, *Light is a Messenger: The life and science of William Lawrence Bragg* (Oxford: Oxford University Press, 2004), 70 and 104.

<sup>41</sup>Darwin came back to Cambridge after the war and was made a fellow of Christ's College while G.P. was a fellow in Corpus Christi. On Darwin, see George P. Thomson, "Charles Galton Darwin" *Biographical Memoirs of Fellows of the Royal Society* 9 (1963), 69–85.

<sup>42</sup>The following anecdote helps to illustrate the importance of electromagnetic deflection. Probably around the beginning of March 1928, he also had the opportunity to discuss his experimental results with Schrödinger himself as the latter recalled in 1945: "After mentioning briefly the new theoretical ideas that came up in 1925/26, I wish to tell of my meeting you in Cambridge in 1927/28 (I think it was in 1928) and of the great impression the marvellous first interference photographs made on me, which you kindly brought to Mr Birthwistle's house, where I was confined with a cold. I remember particularly a fit of scepticism on my side ("And how do you know it is not the interference pattern of some secondary X-rays?") which you immediately met by a magnificent plate, showing the whole pattern turned aside by a magnetic field." Schrodinger to G.P. Thomson, 5th February 1945, George P. Thomson Archives, Trinity College, Cambridge, J105, 4. The exact date can be traced by the minutes of the Kapitza Club, which says that Schrödinger gave a paper to the Club on March 10th, 1928. See *Churchill Archives*, CKFT, 7/1.

<sup>43</sup>George P. Thomson, op. cit. (38), I, 608.

<sup>44</sup>*Ibid.*, 608–609.

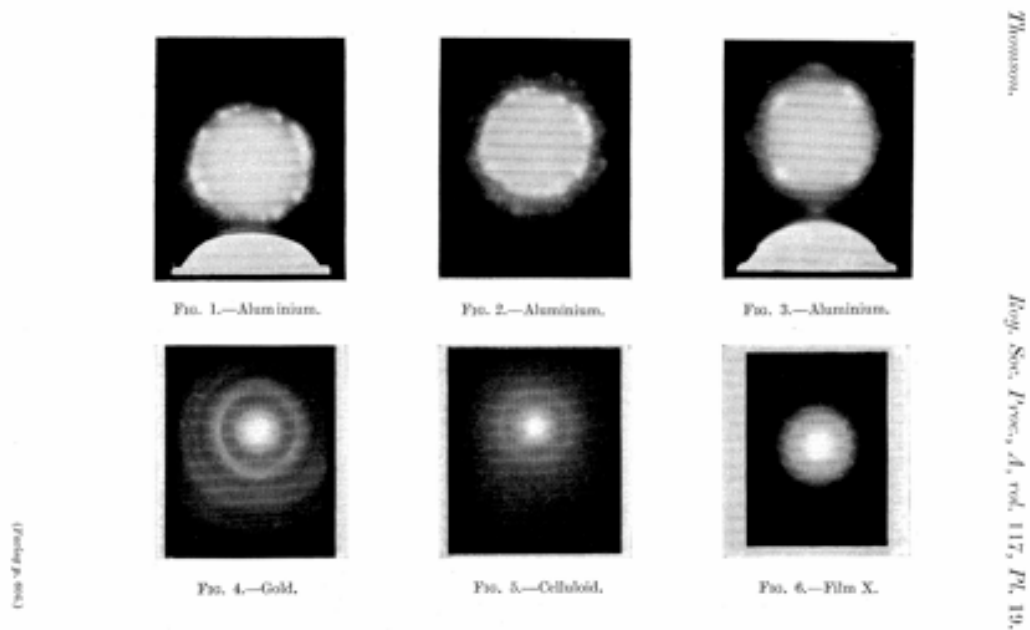


Figure 12.3: Pictures from G.P.’s experiments on electron diffraction.

might want to consider when and how G.P. got in touch with the latest developments going on in Copenhagen.

Besides the impetus that the BAAS Oxford meeting of 1926 meant for many British physicists, G.P. benefited, once again, from his close friendship with C. G. Darwin who, since 1924 the Tait Professor of Natural Philosophy in Edinburgh, spent two months in Copenhagen in the spring of 1927, where he learned about the latest developments in quantum physics and complementarity from Bohr and Heisenberg themselves. On his way back, Darwin spent some time in Aberdeen, in G.P.’s home. This way, G.P. learned all about it from Darwin’s explanations: “we had long talks about all this, and really began to get an idea about it”.<sup>45</sup> The timing was just right. As G.P. was seeing with his own eyes the diffraction patterns of cathode rays, he understood their importance in the context of the latest theoretical developments of quantum mechanics from possibly the British physicist best suited for understanding them at the moment. In his biographical memoir on Darwin, G.P. said that “I am inclined to think that his most useful work was as an interpreter of the new quantum theory to experimental physicists. (...) I should like to record my great debt to him for the many ideas in physics he helped me to understand”.<sup>46</sup>

The pictures convinced G.P. of the validity of de Broglie’s principle. But contrary to what had happened in 1925 when he first learnt about the new theory, G.P. was no longer interpreting it in terms of his father’s metaphysical framework. In the last section we will explore the change of mindset that can be perceived in the early explanations about electron diffraction that G.P. gave, and the uses he made of it. However, let’s

<sup>45</sup>Oral interview with G.P. Thomson, *Archive for the History of Quantum Physics*, Tape T2, side 2, 15.

<sup>46</sup>George P. Thomson, op. cit. (41), 81.

pause for a moment before that and look at the reaction of his father, J.J., in the face of the unavoidable experimental evidence.

## J.J.'s reaction

The father saw, in the experiments of his son, the final proof of his life-long metaphysical project and a clear sign of the invalidity of quantum physics as an ultimate explanation. His world had always been, and still was, a world of ether, in which discrete entities, including the electrons, were but epiphenomena in the ether. Now, in 1928, J.J. Thomson felt his metaphysical idea had proved true and that electron diffraction was a sign that discrete models of matter were only rough approximations to reality. In his mind, the “very interesting theory of wave dynamics put forward by L. de Broglie”, and experimentally proved by his son, was not in contradiction with classical mechanics. In the first of a series of papers he would publish in *Philosophical Magazine*, J.J. tried to show that “the waves are also a consequence of classical dynamics if that be combined with the view that an electric charge is not to be regarded as a point without structure, but as an assemblage of lines of force starting from the charge and stretching out into space”.<sup>47</sup>

Thomson had never accepted the idea put forward by Larmor and Lorentz at the turn of the century of an electron being a point charge of electricity in the ether. Now, the detection of a train of waves associated with the movement of electrons was proof that he had been right: Maxwell's equations had not predicted such a wave for a point electron, and *therefore* such a view of the electron had to be wrong. On the other hand, de Broglie's wave could be obtained on purely classical grounds if he assumed the electron to be a two-part system: a “nucleus which (...) is a charge  $e$  of negative electricity concentrated in a small sphere”,<sup>48</sup> and a sphere surrounding it “made up of parts which can be set in motion by electric forces (...) consist[ing] either of a distribution of discrete lines of force, or of a number of positively- and negatively-electrified particles distributed through the sphere of the electron”.<sup>49</sup> With this *ad hoc* structure J.J. deduced the relationship between the speed of an electron and the wavelength of its sphere to be the same as that expected by de Broglie and measured by G.P.

In a conference given in Girton College, Cambridge, in March 1928 entitled *Beyond the Electron*, J.J. argued that talking about a structure for the electron was not ludicrous. Thirty years earlier, when he first suggested that corpuscles would be constituents of all atoms, thus initiating the exploration of the structure of the atom, he had been accused of being an alchemist. The developments of the physics of the electron had dismissed that accusation. Now he felt justified to talk about the structure of the electron in the light of the latest developments by his son. “Is not going beyond the electron really going too far, ought one not draw the line somewhere?”, he would ask rhetorically. To

---

<sup>47</sup> Joseph J. Thomson, “Waves associated with Moving Electrons” *Philosophical Magazine* 5 (1928), 191–198, 191.

<sup>48</sup> Joseph J. Thomson, “Electronic Waves and the Electron” *Philosophical Magazine* 6 (1928), 1254–1281, 1259.

<sup>49</sup> *Ibid.*, 1254. J.J.'s model for the electron sphere would soon be expressed in terms only of what he came to call “granules”, particles “having the same mass  $\mu$ , moving with the velocity of light  $c$ , and possessing the same energy  $\mu c^2$ ”. See Joseph J. Thomson, “Atoms and Electrons” *Manchester Memoirs* 75 (1930–31), 77–93, 86.

which he would reply that “It is the charm of Physics that there are no hard and fast boundaries, that each discovery is not a terminus but an avenue leading to country as yet unexplored, and that however long the science may exist there will still be an abundance of unsolved problems and no danger of unemployment for physicists”.<sup>50</sup>

The diffraction experiments showed that “we have energy located at the electron itself, but moving along with it and guiding it, we have also a system of waves”.<sup>51</sup> Following the similarities with his structure of light of 1924, he supposed that the electron “had a dual structure, one part of this structure, that where the energy is located, being built up with a number of lines of electric force, while the other part is a train of waves in resonance with the electron and which determine the path along which it travels”.<sup>52</sup> For him, the association of a wave with an electron was not a new phenomenon. It had already happened when, in the late 18th century, the corpuscles of light that Newton had postulated needed to be complemented by wave explanations. It was not so strange to see that the new corpuscles, the electrons, had to undergo a similar process. Furthermore, discussions on the nature of light in the previous two decades had paved the way for the acceptance of the duality of the electron.

In the world of J.J, electron diffraction brought with it the possibility of challenging, rather than accepting, the new quantum physics. A continuous metaphysics in which all phenomena and entities could be seen as structures of the ether was, in his view, still possible. Furthermore, J.J. felt that at last electron diffraction provided the final argument to defend the old worldview, something that the developments of the previous two decades had, only apparently, jeopardised. Electron diffraction was proof of the complexity of the electron and, therefore, of the validity of classical mechanics. Quantification of magnitudes such as momentum or energy “is the result and expression of the structure of the electron; only such motions are possible, or at any rate stable, as are in resonance with the vibrations of the underworld of the electron”.<sup>53</sup>

At the root of his models there was a metaphysical problem as much as an epistemological one. As already stated, J.J.’s metaphysics involved a continuum in terms of which all discrete phenomena could, and should, be explained. Parallel to that was an epistemological problem: for Thomson, de Broglie’s and Schrödinger’s theories, as much as Planck’s, were valid only from a mathematical point of view. Their results were valid, but they did not entail real, true physics. And that was the strength J.J. saw his theory had over de Broglie’s: “The coincidences are remarkable because two theories could hardly be more different in their points of view. M. de Broglie’s theory is purely analytical in form; the one I have brought before you (...) is essentially physical”.<sup>54</sup> It comes to no surprise that, true to the spirit in which he was educated in the old Mathematical Tripos, physical meant mechanical.

In an ironical remark on the situation of physics in previous years he would state in 1930 that “when the waves are taken into account, the classical theory of dynamics gives the requisite distribution of orbit [of the electrons] in the atom, and as far as these go the properties of the atom are not more inconsistent with classical dynamics than are the properties of organ pipes and violin strings, in which, as in the case of the electron,

---

<sup>50</sup>J.J. Thomson, *Beyond the Electron* (Cambridge: Cambridge University Press, 1928), 9.

<sup>51</sup>*Ibid.*, 22.

<sup>52</sup>*Ibid.*, 23.

<sup>53</sup>*Ibid.*, 31.

<sup>54</sup>*Ibid.*, 34.



waves have to be accommodated within a certain distance. It is too much to expect even from classical dynamics that it should give the right result when supplied with the wrong material".<sup>55</sup> Obviously, the fact that the proof had come in the family was only an added reason to rejoice.<sup>56</sup> In the decade between these events and his death in 1940, J.J. did not change his mind. The last paper he ever published, sent in October 1938 at age 81, still reclaimed his son's experiments as proof of the validity of the old classical mechanics.

## G.P.'s evolution

G.P. presented his first preliminary results in a short note in *Nature* dated May 1927 and in a presentation at the Kapitza Club, in Cambridge, on the 2nd of August.<sup>57</sup> In November he was ready to publish a long and detailed paper in the *Proceedings of the Royal Society* preceded by another short note in *Nature*.<sup>58</sup> Although these papers are basically a cold description of the experimental methods and results, some distance from his father's metaphysics is already apparent. As noted above, G.P. realised that his experiments meant a proof of de Broglie's principle and, *therefore*, undermined the validity of classical mechanics. In his words, his experiments involved "accepting the view that ordinary Newtonian mechanics are only a first approximation to the truth (...). However difficult it may seem to accept such a sweeping generalisation, it seems impossible to explain the results obtained except by the assumption of some kind of diffraction".<sup>59</sup>

For the first time in his career we can see a strong contrast between his and J.J.'s position. Both father and son accepted the law of de Broglie, but in different terms. The father wanted to obtain the same relationship between speed, mass and wavelength of the electron by creating an *ad hoc* mechanical model; the son saw the incompatibility of both approaches and opted for a correspondence between the old and the new, between Newton and de Broglie, in terms advocated by Bohr and the school of Copenhagen. G.P. was cutting the umbilical cord that had kept him tied to his father and to the old worldview for far too long.

But this change was no easy business. Two basic questions were at stake: the relationship between the particle and the wave associated with it, and the nature of the medium in which these waves propagate. Before turning to his answer to these questions, we should reflect on G.P.'s attitude towards experimental and theoretical science. A quotation from his Friday speech at the Royal Institution of 1929 describes his approach to theoretical speculation in this period of his life. After explaining with full detail the experiments on electron diffraction he would venture into trying to answer the "great difficulties of interpretation. What are these waves? Are they another name for the electron itself? (...) Some of these questions I should like very briefly to discuss, but we now leave the sure foothold of experiment for the dangerous but fascinating paths

---

<sup>55</sup> Joseph J. Thomson, *Tendencies of recent investigations in the field of Physics*, (London: British Broadcasting Corporation, 1930), 26–27.

<sup>56</sup> Oral interview with G.P. Thomson, *Archive for the History of Quantum Physics*, Tape T2, side 2, 9: "Well, I think he was very pleased [with my developments], largely because it was in the family".

<sup>57</sup> Thomson and Reid, op. cit. (37), and *Churchill Archives*, CKFT 7/1.

<sup>58</sup> George P. Thomson, op. cit. (38).

<sup>59</sup> George P. Thomson, op. cit. (38), I, 608–609.

traced by the mathematicians among the quicksands of metaphysics”.<sup>60</sup> The contrast between the security of experimental data and the uncertainty of theorising is, in this quotation, very strong, and shows how G.P. was sticking to what he considered to be the facts, and distrusting unnecessary speculation.

This speech is also the first time in which he publicly and explicitly distances himself from his father’s ideas. Contrary to J.J.’s explanation of the electron waves in terms of a modification of the ether, G.P. dismisses the need of an ether and takes, for the first time, a pragmatic and positivistic stand. “Personally—he says—I see no necessity for there to be any vibration of a material or quasi-material object. (...) The easiest way of looking at the whole thing seems to be to regard the waves as an expression of the laws of motion”.<sup>61</sup> And to give authority to his point of view, he finished his speculations by quoting Newton’s famous ‘hypothesis non fingo’.

The best and most exhaustive document we have to understand G.P.’s views at the time of his experiments is a series of lectures he gave at the University of Cornell the last term of 1929, and immediately published in the form of a book, *The Wave Mechanics of Free Electrons*. Here we find a thorough explanation of the reasons why he wanted to avoid the question of the ether. The wave-lengths of electron waves and X-rays are in the same range, but they clearly behave differently, for the first can be deflected, and the second can’t. If that is the case, one might need to assume two different media to account for the different behaviour of the two waves, “but it is not a very attractive idea to have two ethers filling the space, especially as the waves of protons—if they exist—would demand yet a third. Space is becoming overcrowded”.<sup>62</sup> G.P.’s decision was to apply Ockham’s razor, to do away with the ether and stick to the information given by the wave formulation, and “perhaps simple physicists may be content as long as the waves do their job guiding the electron, and it is possible that, after all, the question will ultimately be seen to be meaningless”.<sup>63</sup> G.P. seems to be here in close agreement with the spirit of the Copenhagen Interpretation, mixing epistemology and metaphysics, and reducing what there is to what can be described.

One of G.P.’s most surprising speculations in these years was his adherence to the possibility, put forward by Bohr, that energy conservation might have to be abandoned in order to explain beta radioactive decay.<sup>64</sup> Closely following calculations made by his friend Darwin on his way back from Copenhagen, G.P. suggested a mechanism to account for the dispersion of energy. Essentially, G.P. was suggesting that the actual beta emission did conserve energy, only that the huge acceleration suffered by the electron in its ejection from the nucleus involved the creation of an energetic wave, like “the sound produced by the firing of an atomic gun whose bullet is the electron”.<sup>65</sup> Such a wave could be supposed to “possess energy when highly concentrated which it loses on spreading out,”<sup>66</sup> giving rise to an indeterminacy in the energy of the electron. The

---

<sup>60</sup>George P. Thomson, “The Waves of an Electron” *Nature* 122 (1928), 279–282, 281.

<sup>61</sup>*Ibid.*, 282.

<sup>62</sup>George P. Thomson, *The Wave Mechanics of Free Electrons* (New York & London, 1930), 11.

<sup>63</sup>*Ibid.*, 12.

<sup>64</sup>For a thorough analysis of the problems with beta decay and the conservation of energy, see Carsten Jensen, *Controversy and Consensus: nuclear beta decay, 1911–1934* (Basel: Birkhäuser, 2000).

<sup>65</sup>George P. Thomson, “On the Waves associated with  $\beta$ -Rays, and the Relation between Free Electrons and their Waves” *Philosophical Magazine* 7 (1929), 405–417, 410.

<sup>66</sup>*Ibid.*, 415.

actual mechanism G.P. was thinking of was based on basic mathematical properties of waves: the Fourier transformation of the initial pulse would give all possible monochromatic wavelengths and, therefore, all possible energies. The emitted electron would choose only one of these monochromatic waves, thus explaining the indeterminacy in their energy.<sup>67</sup> G.P. did not follow this idea any further since he was step-by-step coming to understand that the new physics was totally alien to the old notion of explanation by way of mechanical models.

As for the relationship between the wave and the particle, the question arises as to which is the *real* thing. Here his position is less clear, but there doesn't seem to be a total identification of both. The wave *guides* the electron but is not totally identifiable with the electron, since what one really observes is the particle, not the wave: "Whenever an electron produces any detectable effect it does so as a particle, and it seems easiest to suppose that even when it is not producing an effect the particle is somewhere round".<sup>68</sup> An example he would often use in his popular lectures is that of the gossamer spider:

"When at rest this spider is a minute insect. When it wants to move it sends out streamers into the air, and floats away owing to the action of the air on these filaments which stretch out a foot or more all round it. Just so the electron, when it is part of an atom its waves are limited to that atom, or even to a part of it. They are curled round on themselves, as it were. Suppose, now, an electron escapes from the hot filament of a wireless valve and gets free. Its waves will spread far out into the space round it. I regard it as still a particle at the centre of its wave system. The analogy can be pressed further. If the wind sweeps the spider past an obstacle the filaments will catch. The pull on filaments will move the spider, and he will feel that there is something in the way, even though his body does not actually hit it. In the same way the waves are a means by which the motion of the electron is affected by things which the main body of the electron never comes very near".<sup>69</sup>

The Aberdeen experience came to an end in 1930, when he was offered the chair at Imperial College, London, after his close friend W.H. Bragg had declined the offer. In his new appointment, G.P. made use of his experimental skills to study the minutiae of electron diffraction and some possible applications, soon to move, following the steps

---

<sup>67</sup>See George P. Thomson, "The Disintegration of Radium E from the Point of View of Wave Mechanics" *Nature* 121 (1928), 615–616: "[The apparent non conservation of energy] is to be expected on the new wave mechanics, if the ejection of a  $\beta$ -particle is produced by anything like a sudden explosion. In such a case one would expect that the wave-group which accompanies, and on some views actually constitutes, the electron, would be of the nature of a single pulse, that is, the damping factor of the amplitude would be of the order of the wave-length. Such a wave-group, being very far from monochromatic, would spread rapidly lengthwise owing to the large dispersion of the phase waves, and so the distance within which the electron may occur becomes large, implying a marked 'straggling' in velocity. Similarly, if the waves pass through a magnetic field, which is for them a refracting medium, the group will split into monochromatic waves going in different directions, just as white light is split up by a prism. Thus an observer who forms the magnetic spectrum of the  $\beta$ -rays will find electrons in places corresponding to paths of various curvatures, that is, he will find a spectrum continuous over a wide range".

<sup>68</sup>George P. Thomson, *op. cit.* (62), 10.

<sup>69</sup>George P. Thomson, "New Discoveries about Electrons" *The Listener* 1 (1929), 219–220, 220.

of Fermi, to the more fashionable and very promising field of slow neutrons. Electron diffraction, for which he would become universally known and receive the Nobel Prize in 1937, soon became a closed chapter of his scientific life.

### Conclusion

A textbook history of the early developments of quantum physics will, at most, only contain a footnote mentioning G.P.'s experiments on electron diffraction. And certainly no reference will be made to the antagonism and speculations of J.J. Thomson. However, a good history of quantum physics should analyse the attitudes, ideas and reactions of both the 'winners' and the 'losers', to avoid being whiggish. J.J. Thomson can be considered to be one of such losers; but in the 1920s he was still a public icon of British science. True, he didn't play a major role at the forefront of science, but he was a very influential figure among second line scientists and the general public. The study of his reaction against quantum physics is certainly necessary if we want to understand the public perception of quantum physics in the 1920s.

At a less social level, one can also use this case study as a way to analyse the role that experimental physics played in the configuration and acceptance of quantum physics. Electron diffraction was proof that electrons behaved like waves, and it triggered in G.P. a certain conviction that wave mechanics, with all the epistemological implications, was worthwhile embracing. But, as we have seen, the experiments were not necessarily an *experimentum crucis* for wave mechanics, certainly not for J.J. and his generation, who were, in Kuhnian terms, excessively immersed in the paradigm of ether physics.<sup>70</sup> This case study reveals the complexities in interpreting experimental results. The same experiments triggered different, almost opposite, responses in the father and in the son.

---

<sup>70</sup>The antagonism to quantum mechanics was not exclusive to Cambridge. In Oxford, for instance, the head of the Clarendon Laboratory stubbornly rejected quantum physics. See Benoit Lelong, "Translating Ion Physics from Cambridge to Oxford: John Townsend and the Electrical Laboratory, 1900–24", in *Physics in Oxford 1839–1939. Laboratories, Learning and College Life*, ed. Robert Fox and Graeme Gooday (Oxford: Oxford University Press, 2005), 209–232, 229: "The break of international physics became more marked after the war. Townsend first ignored and then rejected the emerging quantum theories".



# 13 Weyl Entering the 'New' Quantum Mechanics Discourse

ERHARD SCHOLZ

*Early in 1925 H. Weyl finished his great series of publications on the representation of Lie groups and started the studies for his Philosophie der Mathematik und Naturwissenschaften delivered to the editors in summer 1926. He was in touch with M. Born and got to know of the developments in the Göttingen group around Born, Heisenberg and Jordan in early summer 1925. After a conversation with Born in September 1925 he started to develop ideas of his own how to quantize the mechanical observables of a system and communicated them to Born and Jordan in October 1925. In these letters he proposed the basic idea of a group theoretic approach to quantization, which he presented to the scientific public in his 1927 paper Quantenmechanik und Gruppentheorie. This paper had a long and difficult reception history for several decades.*

## Introduction

There are many stories to be told about Hermann Weyl's involvement in quantum mechanics. Among them:

- 1918–1923, Weyl's rising awareness of the role of quantum structures in the constitution of matter during his phase of a dynamistic matter explanation in the frame of the Mie-Hilbert-Weyl program,<sup>1</sup>
- 1925–1927, backstage involvement in the new QM leading to his published contribution to the topic Weyl (1927) quoted as QMG in the sequel,
- 1927/28 lecture course and book publication on *Groups and Quantum Mechanics*, quoted as GQM,
- 1929, Weyl's contribution to the general relativistic Dirac equation (Fock-Weyl theory),
- 1930ff. study of the role of spin coupling for molecular bounds, second edition of GQM, and later contributions.

This is too much for a conference talk. Here I shall concentrate on the second item. For items 4 see Scholz (2005), for 3 and 5 Scholz (2006), for item 1 with a link to 4 Scholz (2004a,b).

---

<sup>1</sup>This relates to Weyl's role in the *Forman thesis*. P. Forman's version should not be taken literally, however, and has to be reconsidered and drastically corrected.

The reason for this choice is that Weyl's contributions to QM during the period 1925–1927 may be of particular interest for this conference. It contains a direct communication between him and two of the main protagonists of the 'new' quantum mechanics, Max Born and Pascual Jordan, in late summer and early autumn 1925. Moreover we find here a *very early* formulation of a structural approach to quantization. This may be helpful to understand historically, and perhaps more widely, a mathematician's view of the relationship mathematics—physics in foundational aspects.<sup>2</sup>

During the years 1924 and 1925 Weyl worked hard on his great series on the representation theory of Lie groups, beautifully described in Hawkins (2000). It was finished in April 1925 Weyl (1925/1926). Then he started intense reading work for his contribution to *Philosophie der Mathematik und Naturwissenschaften in Handbuch der Philosophie*. He took this task very seriously; it occupied him well into the year 1926. In his letter to Born of Sep. 27, 1925, he characterized himself as “fettered to the deep swamp of philosophy (gefesselt an das tiefe Moor der Philosophie)”. This did not hinder him, on the other hand, to follow very closely what was going on inside the Göttingen group of theoretical physics during 1925, with its great step towards a new kind of mathematized quantum mechanics.

Already earlier in the 1920s, Weyl had found two topics in modern physics, in which group representations became important. The first topic was in general relativity and differential geometry. The representation theory of the special linear group  $SL_n\mathbb{R}$ , showed that there is a *mathematical reason for the structural importance of tensors in differential geometry*.<sup>3</sup> The second point became clear to him, when Elie Cartan proved that the algebraic part of Weyl's *analysis of the space problem* could be answered by the use of group representations more easily.<sup>4</sup>

When Weyl learned from M. Born in September 1925 of the recent Göttingen work in quantum mechanics, he immediately tried to link the new theory to the representation theory of groups. Already in autumn 1925 he started to investigate in how far group representations might help to understand the Göttingen quantization procedure and, in particular, how they shed light on the role of the Heisenberg commutation rule (section 2 below). His approach led directly to the study of abelian ray representations. He even made first steps towards what later turned into Weyl quantization (section 3). Both ideas were first published in QMG Weyl (1927). This contribution ends with some remarks on Weyl's indications on interacting and/or relativistic systems (section 4) and a short outlook on reception and repercussions of Weyl's proposals (section 5).

## From Commutation Rules to Abelian Ray Representations

Shortly before leaving for a visit to the US of America, Max Born visited Zürich in September 1925 and informed Weyl on the recent progress in QM made at Göttingen. This led to a short correspondence between Born and Weyl (Weyl to Born Sept. 27, 1925,

---

<sup>2</sup>Here “foundational” is understood in the sense of foundations of physics, not as foundations of mathematics.

<sup>3</sup>All irreducible representations of  $SL_2\mathbb{R}$ , arise as subrepresentations of tensor products of the natural representation with certain symmetry properties. Thus infinitesimal structures of classical differential geometry have a good chance to be expressible in terms of vector and tensor fields.

<sup>4</sup>Hawkins (2000); Scholz (2004b)

Born to Weyl Oct. 3, 1925) and, after Born's departure, between Weyl and Jordan (Weyl to Jordan Oct. 13, 1925, Jordan to Weyl, Nov. 1925, and two postcards, Weyl to Jordan, Nov. 23 and 25, 1925). The correspondence took place in the time lapsed between the submission and publication of Born's and Jordan's common article on quantum mechanics Born (1925).<sup>5</sup>

Apparently Born had explained the content of this paper to Weyl. The latter wrote to Born:

Dear Herr Born!

Your Ansatz for quantum theory has impressed me tremendously. I have figured out (zurecht gelegt) the mathematical side of it for myself, perhaps it may be useful for your further progress ... Weyl (Ms1925a).<sup>6</sup>

In his "Zurechtlegung des Mathematischen" Weyl immediately passed over from the *matrices*  $p, q$  etc. of Born, Heisenberg, and Jordan to the "one-parameter group which results from the infinitesimal transformation  $1 + \delta p$  by iteration" (the  $\delta$  was introduced by Weyl to characterize the limit process  $\delta p$  for  $\delta \rightarrow 0$ ),

$$P(s) = e^{ps} = 1 + sp + \frac{s^2}{2!}p^2 \dots, \quad Q(t) = e^{qt} = 1 + tq + \frac{t^2}{2!}q^2 \dots \quad (s, t \in \mathbb{R}).$$

That is, he considered the  $p, q$  as *infinitesimal generators of 1-parameter groups*. He did not touch analytical details of domains of definition etc..<sup>7</sup>

This move was motivated by Weyl's recent experiences with Lie groups. There he had studied the consequences of the shift from the infinitesimal group (now, Lie algebra) to the finite one (the Lie group itself) for the corresponding representations. He had found valuable new insights by such a shift from the infinitesimal to the integral (finite) point of view.

In the context presented to him by Born, Weyl realized that the Heisenberg commutation rule for the infinitesimal operators

$$pq - qp = \hbar 1, \tag{13.1}$$

with  $\hbar$  "a number" (Weyl omitted the imaginary unit  $i$ ), was (and is) equivalent to the quasi-commutation rule for the integral operators  $P := P(1), Q := Q(1)$

$$PQ = \alpha QP, \quad \text{with } \alpha(s, t) \text{ complex factor.} \tag{13.2}$$

This looked like an easy reason for the validity of Heisenberg commutation in quantum mechanics, where states were represented by functions or vectors up to a non-vanishing complex factor only, if normalized up to a phase factor  $\alpha$ ,  $|\alpha| = 1$ , "... which one [could] deny any physical meaning" (Weyl Ms1925a). In this sense the integral version (2) of

<sup>5</sup>Submission date, 27 Sept., publication 28 November 1925.

<sup>6</sup>The German original is even nicer: "Lieber Herr Born, Ihr Ansatz zur Quantentheorie hat auf mich gewaltigen Eindruck gemacht. Ich habe mir das Mathematische dazu folgendermaßen zurecht gelegt, vielleicht kann Ihnen das bei 'der weiteren Durchführung behülflich sein ..."

<sup>7</sup>This state of affairs pertained well into 1927. Even Hilbert in his lecture course in winter semester 1926/27 and did not specify domains of definition. This situation started only to be changed with von Neumann's first own contribution on the foundations of QM.



Zürich, d. 27. Sept. 25.  
Bolligenstr. 52

Lieber Herr Born!

Ihre Ansicht zur Quantentheorie hat auf mich gewaltigen Eindruck gemacht. Ich habe mich der mathematischen dazu folgendermaßen gewacht gelehrt, vielleicht kann Ihnen das bei der weiteren Durchführung noch behilflich sein. Sind  $p, q$  Matrizen,  $e$  die Einheitsmatrix,  $\delta, \varepsilon$  unendlichkleine Zahlen, so gilt für den Kommutator  $PQ - QP = \hbar$  der beiden infinitesimalen Transformationen

$$P = e + \delta p, \quad Q = e + \varepsilon q$$

$$PQ - QP = \hbar + \delta\varepsilon \{pq - qp\} + \text{Glieder, die mit } \delta \rightarrow 0, \varepsilon \rightarrow 0 \text{ zu } 0 \text{ konvergieren}$$

In Ihrem Fall, wo  $pq - qp = \hbar \cdot e$  ( $\hbar$  eine Zahl)

gilt demnach  $PQ = \alpha QP$ , wo  $\alpha = 1 + \hbar\delta\varepsilon$ .

Nun folgt aus einer solchen Gleichung sofort

$$P^n Q^n = \alpha^{n^2} Q^n P^n$$

Wenn wir hier  $n = \frac{1}{\delta\varepsilon}$  die willkürliche Zahl  $\frac{1}{\delta\varepsilon}$  setzen, so schreiben wir

$$e^{\xi p} e^{\eta q} = e^{\hbar \xi \eta} e^{\eta q} e^{\xi p}$$

wo  $e^{\xi p} = e + \frac{\xi p}{1!} + \frac{\xi^2 p^2}{2!} + \dots$  gesetzt ist (die eisensteinische Gruppe, die aus der inf. Transf.  $e + \delta p$  durch Potenzieren entspringt). Diese Gleichung faßt, wenn man links und rechts das Glied  $e^{\eta q}$  verfrachtet, die Potenzen  $p^i q^k$  bequemer zusammen. Betrachtet man insbesondere links und rechts das Glied mit  $\xi$ , bezw. mit  $\xi^r$ , so kommt

$$p e^{\eta q} = e^{\eta q} (p + \hbar \eta)$$

Bei der Definition  $f_p = \eta p^{m-1} q^n$ ,  $f_q = \eta p^m q^{n-1}$  für  $f = p^m q^n$  liefert die erste für  $f = e^{\xi p} e^{\eta q}$  die Formel

$$p \cdot f - f \cdot p = \hbar f_q$$

Figure 13.1: Weyl to Born, 27 Sept. 1925, page 1

the commutation rule seemed more basic to Weyl. He started to explore first conclusions of it for algebraic expressions of  $p$  and  $q$ , which we do not go into here (we come back to this question in the discussion of Weyl's letter to Jordan).

Born's reaction was polite,

Dear Herr Weyl,

It was a great pleasure for me to see that our new quantum mechanics attracts your interest. In the meantime, we have made considerable progress and are now sure that our approach covers the most important aspects of the atomic structure. . . . Born (Ms 1925)

But apparently he was not particularly interested in Weyl's proposal. In the last phrase Born referred to his joint paper with Jordan, just submitted to *Zeitschrift für Physik*. Then he continued:

It is very fine that you have thought about our formulas; we have derived these formulas in our way, even if not as elegantly as you, and intend to publish the subject in this form, because your method is difficult for physicists to access. (ibid)<sup>8</sup>

So Weyl was left alone with his proposal to pass over to the integral version of the infinitesimal transformations.

He saw the opportunity to come back to the question in a direct communication with the younger colleague a little later. On 13 Nov. 1925 he received proofs of Born and Jordan's paper, "against acknowledgement of receipt and by express mail! (eingeschrieben und durch Eilboten!)", as he remarked with some surprise in his first letter to Jordan. He did not go into the details of the paper but referred to his letter to Born, in which he had done some of the calculations in his own approach, and added some other comments.

Jordan replied in November (no day specified in the date) answering that he had seen Weyl's letter to Born. But also he did not take up the idea of passing to the one-parameter integral groups.<sup>9</sup> He added that in the meantime he and Born had found their own way to establish the Heisenberg commutation relation "*without* any other precondition" from the "equations of motion"

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}$$

for a Hamilton operator  $H$  which could be expressed algebraically by a polynomial in  $p$  and  $q$ .

In a footnote he added

---

<sup>8</sup>"Lieber Herr Weyl,

daß unsere neue Quantenmechanik Ihr Interesse erregt, hat mir große Freude gemacht. Wir sind inzwischen sehr viel weiter gekommen und sind jetzt ganz sicher, daß unser Ansatz die wesentlichen Züge der Atomstruktur richtig trifft. Daß Sie sich selbst mit unsern Formeln beschäftigt haben, ist sehr schön; wir haben diese Formeln uns auch, wenn auch nicht so elegant, hergeleitet und werden wohl in dieser Form die Sache veröffentlichen, weil Ihr Verfahren für die Physiker wohl zu schwer ist. . . ." Born (Ms 1925)

<sup>9</sup>"Ihren Brief an Prof. Born habe ich seinerzeit mit Interesse gelesen . . ." Jordan ( Ms 1925). Apparently Born had handed over the letter to Jordan during the final preparation of the manuscript. It remained in Jordan's hand and is still in his Nachlass (Staatsbibliothek Berlin).

When Born talked to you, we still believed that  $pq - qp = \frac{\hbar}{2\pi i} 1$  is an independent *requirement*.<sup>10</sup>

So, even if Weyl's proposal to consider integral versions of 1-parameter operator groups and their natural quasi-commutation rule (2) did not immediately enter the Göttingen discourse on the foundation of QM, he seemed to have triggered second thoughts of the Göttingen physicists on how to derive Heisenberg commutation from basic principles of QM ("without any other precondition"). Born and Jordan succeeded by referring to the Hamilton operator of the system.

On the other hand, it appeared unnatural for Weyl to consider only polynomial expressions in the basic momentum and localization operators  $p, q$  for  $H$ . In his postcards Weyl mentioned an idea to Jordan, which kind of functions for  $H$  (classical Hamiltonian) might be taken into consideration for a quantum analogue of  $H$ .

I conclude that the domain of acceptable functions  $H$  is characterized by the Ansatz

$$\int \int e^{\xi p + \eta q} \varphi(\xi, \eta) d\xi d\eta. \quad (13.3)$$

This is less formal than  $\sum p^m q^n$  Weyl (Ms1925c) (equ. number added, E.S.).<sup>11</sup>

The formula has to be read with the imaginary unit in the exponential,  $\int e^{i(\xi p + \eta q)}$ . Weyl was used to omit these to "facilitate reading", as he felt.<sup>12</sup> Thus the integral in the postcard to Jordan indicated something like an inverse Fourier transform of  $\varphi$ . It contained the starting point for Weyl's idea of quantization by using operator Fourier integrals. He later explored and extended the idea and published it in 1927 (QMG). We will come back to this point in the next section.

Weyl's idea to look at the operator relations of QM from an integral point of view lay dormant for more than a year. In autumn 1927, shortly before his lecture course on group theory and quantum mechanics started, Weyl finally prepared his article QMG, Weyl (1927).<sup>13</sup> There he discussed some basic principles of the representation of physical quantities in QM by Hermitian forms (in particular simultaneous diagonalizability) as well as the difference of *pure states* (eigenvectors of a typical observable of the system under consideration) and *mixtures* (compositions of pure states in any mixing ratio).<sup>14</sup>

We are here more interested in part two. Weyl announced that this section

... deals with deeper questions. [...]. It is closely connected to the question of the essence and correct definition of a canonical variable. (Weyl, 1927, 92)

<sup>10</sup> "Als Born Sie sprach, glaubten wir noch daß  $pq - qp = \frac{\hbar}{2\pi i} 1$  eine unabhängige *Voraussetzung* sei." Jordan ( Ms 1925) (emphasis in original)

<sup>11</sup> "Ich komme darauf, den Bereich der vernünftigen Funktionen  $H$  durch den Ansatz  $\int \int e^{\xi p + \eta q} \varphi(\xi, \eta) d\xi d\eta$  wiederzugeben; das ist weniger formal als  $\sum p^m q^n$ ."

<sup>12</sup> In a slightly different denotational form: "Um der Leserlichkeit willen schreibe ich oft  $e(x)$  statt  $e^{ix}$ ." (Weyl, 1927, below equ. (35)). In the postcard he even used the exponential form of denotation  $e^{\xi p + \eta q}$  itself.

<sup>13</sup> Submitted October 13, 1927.

<sup>14</sup> Von Neumann characterized mixtures in the same year more precisely by a positive Hermitian operator  $A$  with sum of eigenvalues  $\sum a_\nu = 1$  (trace class operators of trace class norm 1).

He continued by criticizing Jordan's paper (1927) which left "completely unclear" how to assign a matrix  $f(Q)$  to a function  $f(q)$  of position coordinates  $q$ . Moreover Weyl considered Jordan's presentation of the concept of canonical variables "mathematically unsatisfactory and physically unfeasible".

Here I believe to have arrived at a deeper insight into the true state of affairs by the use of group theory. (ibid.)

This insight was gained from extending the approach he had already proposed in his letter to Born in September 1925.

Starting from a Hermitean matrix  $A$ , Weyl associated the corresponding anti-Hermitean

$$C := i A$$

and considered the unitary 1-parameter group generated by it,

$$U(s) = e^{isA} = e^{sC}, \quad s \in \mathbb{R}.$$

For an abelian group  $\tilde{G} = \langle C_1, \dots, C_k \rangle$  generated freely by  $k$  such matrices  $C_1, \dots, C_k$ , he accordingly got a  $k$ -parameter unitary group with typical element

$$U(s_1, \dots, s_k) = e^{i \sum_{\nu} s_{\nu} C_{\nu}}, \quad s \in \mathbb{R}.$$

In QM the commutation of the  $C$ -s and  $U$ -s may be weakened. The weakening of the commutation relation for the unitary group elements

$$U(s)U(t) = U(t)U(s), \quad s, t \in \mathbb{R}^k$$

by admitting phase factors

$$U(s)U(t) = e^{i\alpha(s,t)}U(t)U(s), \quad \alpha(s,t) \in \mathbb{R},$$

corresponded to commutation relations for the generators of the form

$$C_j C_l - C_l C_j = i c_{jl} \cdot 1 \tag{13.4}$$

with skew-symmetric real coefficients  $(c_{jl})$  (*commutator form*).

Weyl argued that for an irreducible group the commutator form is non-degenerate ( $|c_{jl}| \neq 0$ ). By a change of generators it could be normalized to matrix blocks

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

i.e., to the normal form of a symplectic matrix.

For even  $k$ ,  $k = 2n$ , the new generators (after change of base) can be written as

$$iP_{\nu}, \quad iQ_{\nu} \quad (\nu = 1, \dots, n)$$

with  $P_{\nu}, Q_{\nu}$  Hermitian and

$$i(P_{\nu}Q_{\nu} - Q_{\nu}P_{\nu}) = c \cdot 1, \quad c = 1, \hbar. \tag{13.5}$$

All other commutators are 0. By obvious reasons Weyl called  $P_1, \dots, P_n, Q_1, \dots, Q_n$  a *canonical basis* for the representation of  $\tilde{G}$ .

For operators

$$A(s) = e^{i \sum s_\nu P_\nu}, \quad B(t) = e^{i \sum t_\nu Q_\nu}$$

$$W(s, t) := A(s)B(t),$$

the commutation relations acquire the form

$$A(s)B(t) = e^{ic \sum_\nu s_\nu t_\nu} B(t)A(s) \quad (13.6)$$

The commutative addition for  $(s, t), (s', t')$  in  $\mathbb{R}^n$  reappears here slightly deformed as:

$$W(s + s', t + t') = e^{-ic \langle s, t \rangle} W(s, t)W(s', t'), \quad (13.7)$$

where  $\langle s, t \rangle := \sum_\nu s_\nu t_\nu$ .

Weyl called the ‘deformed’ representation

$$\begin{aligned} \tilde{G} := \mathbb{R}^{2n} &\longrightarrow \mathcal{U}(\mathcal{H}) \\ (s, t) &\mapsto W(s, t) = A(s)B(t), \end{aligned} \quad (13.8)$$

with  $\mathcal{U}(\mathcal{H})$  the unitary group of the Hilbert space  $\mathcal{H}$ , an “irreducible group of abelian ray rotations”. Later authors would prefer the terminology *projective (or ray) representation of  $\tilde{G}$* .

Weyl realized that he had found a structural reason, based on group theoretic considerations, for the canonical pairing of basic observables

$$P_\nu, Q_\nu,$$

satisfying the Heisenberg commutation relations

$$[P_\nu, Q_\nu] = -i \hbar 1. \quad (13.9)$$

The latter arose naturally as the infinitesimal counterpart of the integral version for the unitary 1-parameter groups

$$e^{isP_\nu} e^{itQ_\nu} = e^{i\hbar st} e^{itQ_\nu} e^{isP_\nu}, \quad (13.10)$$

with its commutator phase shift  $e^{i\hbar st}$ . In the sequel (13.10) will be called, as usual, the *Weyl commutation relations*.

Weyl showed that in this situation the spectrum of the localization operators  $Q$  was the whole real continuum,  $\mathbb{R}$ , and the pure states could be characterized by square integrable complex-valued functions on  $\mathbb{R}^n =: G$  ( $\tilde{G} = G \times \hat{G}$ , with  $\hat{G}$  dual of  $G$ )

$$\psi \in \mathcal{L}^2(\mathbb{R}^n, \mathbb{C}) \quad \text{of norm } |\psi| = 1$$

on the space of  $q$  localizations. Then the operators (13.8) of the kinematical group  $\mathbb{R}^{2n}$  were represented by translations, respectively phase multiplication operators of the form

$$A(s) \psi(q) = \psi(q - s), \quad B(t) \psi(q) = e^{i \langle t, q \rangle} \psi(q), \quad (13.11)$$

and the canonically paired basis operators became

$$P_\nu : \psi \mapsto i \frac{\partial \psi}{\partial q_\nu}, \quad Q_\nu : \psi \mapsto q_\nu \cdot \psi. \quad (13.12)$$

Weyl commented:

*We have thus arrived at Schrödinger's version* [of quantum mechanics, E.S.].  
(Weyl, 1927, 122, emphasis in original)<sup>15</sup>

In the end, the Schrödinger characterization of a free particle turned out to be nothing but a well chosen basis description of the irreducible ray representation of the non-relativistic kinematical group  $\mathbb{R}^{2n}$ . Moreover, this argument showed that *every irreducible ray representation* of  $\mathbb{R}^{2n}$  was *isomorphic to the Schrödinger picture* of a free particle. Weyl concluded:

*The kinematical character of a physical system is expressed by an irreducible Abelian rotation group the substrate of which* [the set on which it operates, E.S.] *is the ray field (Strahlenkörper) of 'pure cases'.* (Weyl, 1927, 118, emphasis in original)<sup>16</sup>

The “kinematical character” of a non-relativistic quantum system with  $n$  continuous non compactified degrees of freedom turned out to be of a rather simple nature and universally given by the uniquely determined irreducible unitary ray representation of  $\tilde{G}$ .

## Weyl's Approach to the Quantization Problem

We have seen that already in his postcard to P. Jordan Weyl indicated that a Fourier transform kind approach might be helpful to delimit the “domain of reasonable functions  $H$ ” (13.3) or, in slightly more generalized terms, for functions which could be considered as candidates for observables. In his 1927 article Weyl came back to this idea and worked it out in some more detail.

After having arrived at the irreducible ray representation of  $\tilde{G} \cong \mathbb{R}^{2n}$  with canonical basis

$$iP_\nu, iQ_\nu, \quad 1 \leq \nu \leq n,$$

he turned to the interrelation between the quantum system characterized by it and the classical system with  $n$  continuous degrees of freedom, which could be assigned to the former in a natural (structurally well determined) way. The latter had the classical momentum and location observables  $p_1, \dots, p_n, q_1, \dots, q_n$ . Weyl remarked:

A physical quantity is mathematically defined by its functional expression  $f(p, q)$  in the canonical variables  $p, q$ . It remained a problem, how such an expression had to be transferred to the matrices. (Weyl, 1927, 116)<sup>17</sup>

<sup>15</sup> “Damit sind wir bei der Schrödingerschen Fassung angelangt.”

<sup>16</sup> “Der kinematische Charakter eines physikalischen Systems findet seinen Ausdruck in einer irreduziblen Abelschen Drehungsgruppe, deren Substrat der Strahlenkörper der ‘reinen Fälle’ ist.”

<sup>17</sup> “Eine physikalische Größe ist durch ihren Funktionsausdruck  $f(p, q)$  in den kanonischen Variablen  $p, q$  mathematisch definiert. Es blieb ein Problem, wie ein derartiger Ausdruck auf die Matrizen zu übertragen war.”

Weyl reminded the reader that the transfer from classical to quantum observables was clear only for pure monomials of the form  $f(p, q) = p^k$  or  $q^l$ . Already for mixed monomials of the type  $p^2q$  it was no longer uniquely determined how the quantum analogue should be characterized, because of the non-commutativity of Hermitian operators,  $P^2Q, QP^2, PQP$  etc.. To solve this problem he recommended to use Fourier integrals.

Weyl considered the Fourier transform  $\xi$  of  $f$ , normalized like

$$\xi(s, t) = \left(\frac{1}{2\pi}\right)^n \int e^{-i(ps+qt)} f(p, q) d\xi d\eta, \quad \text{in short } \xi = \hat{f},$$

and represented  $f$  as the Fourier inverse of  $\xi$ ,

$$f(p, q) = \int e^{i(ps+qt)} \xi(s, t) ds dt, \quad f = \check{\xi}. \quad (13.13)$$

It appeared rather natural to pass over to the operator analogue

$$\mathcal{F}(f) := \int e^{i(Ps+Qt)} \xi(s, t) ds dt = \int W_{s,t} \xi(s, t) ds dt. \quad (13.14)$$

For a real-valued square-integrable  $f$ , the Fourier transform  $\xi$  is itself square-integrable and satisfies the reality condition

$$\bar{\xi}(s, t) = \xi(-s, -t),$$

which again implies Hermiticity of  $\mathcal{F}(f)$  (Weyl, 1927, 116f.). Weyl therefore considered the resulting  $F := \mathcal{F}(f)$  as a naturally defined quantum mechanical version of the physical quantity related to  $f$ . In the sequel  $\mathcal{F}(f)$  will be called the *Weyl quantized* observable corresponding to  $f$ .

He added:

The integral development (42) [our (13.13), E.S.] is not always to be understood literally. The essential point is only that one has a linear combination of the  $e(p\sigma+q\tau)$  on the right hand side [ $\sigma, \tau$  correspond to our  $s, t$ ,  $e(x) = e^{ix}$ , E.S.], in which  $\sigma$  and  $\tau$  take on arbitrary real values. If, e.g.,  $q$  is a cyclic coordinate which is to be understood mod  $2\pi$  (...), the integration with respect to  $\tau$  becomes a summation over all integer numbers  $\tau$ ; then we have the case of a mixed continuous-discrete group. (Weyl, 1927, 117)<sup>18</sup>

That is, Weyl envisaged the possibility of the torus group and its dual

$$G \cong (S^1)^n =: T^n, \quad \hat{G} \cong \mathbb{Z}^n, \quad \tilde{G} \cong T^n \times \mathbb{Z}^n \quad (13.15)$$

as an example for a mixed continuous-discrete group and considered Fourier integral quantization on it.

---

<sup>18</sup>“Die Integralentwicklung (42) ist nicht immer ganz wörtlich zu verstehen; das wesentliche ist nur, daß rechts eine lineare Kombination der  $e(p\sigma+q\tau)$  steht, in denen  $\sigma$  und  $\tau$  beliebige reelle Werte annehmen können. Wenn z.B.  $q$  eine zyklische Koordinate ist, die nur mod.  $2\pi$  zu verstehen ist, so daß alle in Betracht kommenden Funktionen periodisch in  $q$  mit der Periode  $2\pi$  sind, so wird die Integration nach  $\tau$  ersetzt werden müssen durch eine Summation über alle ganze Zahlen  $\tau$ ; wir haben dann den Fall einer gemischten kontinuierlich-diskreten Gruppe.”

For the existence of the Fourier integral (13.13) Weyl could refer to recent papers by N. Wiener, S. Bochner, G.H. Hardy and J.E. Littlewood on trigonometric integrals.<sup>19</sup> He had thus arrived at a theoretically *satisfying solution of the quantization problem for classical observables* depending only on the kinematical variables  $p$  and  $q$ .

Weyl had now at hand two structurally well defined types of composition of observables on a “kinematical” system, defined by an irreducible ray representation of  $\tilde{G} = \mathbb{R}^{2n}$

- (i) composition of classical “physical quantities”  $f(p, q), g(p, q)$  (real valued functions on  $G$ ) by multiplication,  $f \cdot g$ ,
- (ii) composition of Weyl quantized observables  $\mathcal{F}(f) \circ \mathcal{F}(g)$ , with

$$\begin{aligned} \mathcal{F}(f) &= \int e^{i(Ps+Qt)} \xi(s, t) ds dt \\ \mathcal{F}(g) &= \int e^{i(Ps+Qt)} \eta(s, t) ds dt \quad \text{for } \eta = \check{g}. \end{aligned}$$

Of course these compositions differed essentially, as  $\cdot$  is commutative and  $\circ$  obviously non-commutative. Weyl might have easily transported the operator composition back to the functions on the abelian group, defining  $f * g =: h \iff \mathcal{F}(h) = \mathcal{F}(f) \circ \mathcal{F}(g)$ . But he did not. He was not so much interested in the arising new algebraic structure itself, as in the quantum physical context to which his investigations belonged. The next most pressing problem after the derivation of the Schrödinger representation of a free quantum mechanical system (see above) seemed to be the question, how to characterize interactions, the “dynamical problem” as Weyl called it.

## Reflections on the “Dynamical Problem”

Section III of Weyl’s article dealt with the *dynamical problem*. While the “kinematics” of a system characterized by a continuous group  $G \cong \mathbb{R}^n$  was uniquely determined by its number  $n$  of degrees of freedom, the same did not hold true for the dynamics, taking interactions into account.

Up to now the approach claims general validity. The situation is less comfortable for the *dynamical problem* which is closely bound to the role of *space and time* in quantum physics. (Weyl, 1927, 123, emph. in original)<sup>20</sup>

Weyl immediately hit on a strict limitation for contemporary quantum physics, which was bound to the different roles played by space and time in Galilean and in relativistic quantum physics. In non-relativistic QM, time was an *independent variable*, and even the only one, of a system in the following sense:

Independent variables are no measurable quantities, they are a cognitive spider web of coordinates arbitrarily spread out over the world. The dependence

<sup>19</sup>Wiener (1926); Bochner (1927); Hardy/Littlewood (1926)

<sup>20</sup>“Die bisherigen Ansätze beanspruchen allgemeine Geltung. Nicht so günstig steht es mit dem *dynamischen Problem*, das eng mit der Frage nach der Rolle zusammenhängt, welche *Raum und Zeit* in der Quantenphysik spielen.”



of a physical quantity on these variables can therefore not be controlled by measurement; only if several physical quantities are in play, one can arrive at relations between the observable quantities by elimination of the independent variables. (Weyl, 1927, 124)<sup>21</sup>

Now Weyl indicated a critical difference between field physics and relativistic quantum mechanics on the one side and Galilean QM on the other. Field theory deals with *state quantities* (*Zustandsgrößen*), i.e., observables, which are “spread out in space and time”, while in particle mechanics time may be considered as an independent variable. A relativistic quantum description of the electron, e.g., has to consider spatial coordinates and time as state quantities, “really marked space and, of course, also really marked time” and thus as observables represented by Hermitian forms (or operators).

In contrast to this state of affairs, non-relativistic mechanics is in the comfortable situation to be able to ignore time as a state quantity, while relativistic mechanics needs measurable time coordinates of the particles together with measurable space coordinates. (Weyl, 1927, 124)<sup>22</sup>

The dynamical law of non-relativistic QM could therefore be given in the Schrödinger picture by

$$\frac{d\psi}{dt} = \frac{i}{\hbar} E \cdot \psi$$

(with this sign!), where “ $iE$  is the infinitesimal unitary mapping coupled to the Hermitian form  $E$  which represents energy” (ibid, 124).<sup>23</sup>

For relativistic quantum physics the situation appeared still rather inconclusive, and Weyl indicated only the direction of research one had to pursue:

If one wants to remove the criticized deficiency of the concept of time in the old pre-relativistic quantum mechanics, the measurable quantities time  $t$  and energy  $E$  have to be included as another conjugate pair. This can also be seen from the action principle of analytic mechanics; the dynamical law disappears completely. The relativistic treatment of an electron in the electromagnetic field by Schrödinger e. a. corresponds to this point of view.<sup>24</sup> A more general formulation is not yet available. (Weyl, 1927, 127)<sup>25</sup>

<sup>21</sup> “Die unabhängigen Veränderlichen sind keine gemessenen Größen, sie sind ein willkürlich in die Welt hineingetragenes gedachtes Koordinatenspinngewebe. Die Abhängigkeit einer physikalischen Größe von diesen Variablen ist also auch nicht etwas durch Messung zu Kontrollierendes; erst wenn mehrere physikalische Größen vorliegen, kommt man durch Elimination der unabhängigen Veränderlichen zu Beziehungen zwischen beobachtbaren Größen.”

<sup>22</sup> “Diesem Sachverhalt gegenüber ist die nicht-relativistische Mechanik in der glücklichen Lage, die Zeit als Zustandsgröße ignorieren zu können, während die Relativitätsmechanik parallel mit den meßbaren Raumkoordinaten auch die meßbaren Zeitkoordinaten der Teilchen benötigt.”

<sup>23</sup> Apparently Weyl followed here (Schrödinger, 1926, 142).

<sup>24</sup> Weyl quoted (Schrödinger, 1926, 163ff.).

<sup>25</sup> “Will man den gerügten Mangel des Zeitbegriffs der alten vorrelativistischen Mechanik aufheben, so werden die meßbaren Größen: Zeit  $t$  und Energie  $E$ , als ein weiteres kanonisches Paar auftreten, wie ja bereits das Wirkungsprinzip der analytischen Mechanik erkennen läßt; das dynamische Gesetz kommt ganz in Fortfall. Die Behandlung eines Elektrons im elektromagnetischen Feld nach der Relativitätstheorie durch Schrödinger u. a. entspricht bereits diesem Standpunkt. [Fussnote mit Hinweis auf (Schrödinger, 1926, 163ff.)] Eine allgemeinere Formulierung liegt noch nicht vor.”

“Inclusion” of time and energy as another canonical pair of variables for a relativistic approach would surely imply to take care also for the relativistic transformations between different observers, i.e., the consideration of a ray representations of the Poincaré group with conjugate pairs of translation variables  $(\mathbb{R}^4 \times \mathbb{R}^4) \times SO(1, 3)$  (with  $\times$  for the semi-direct product). However, Weyl left it with the indication quoted above. It would be taken up only much later by E. Wigner and G. Mackey.

In 1927, and still in summer 1928, Weyl apparently hoped that the group theoretic approach might be a guide to field quantization also, at first in the non-relativistic case, but then perhaps even in the relativistic one. At the end of §44 of the first edition of GQM in which he sketched the quantization of the wave equation according to Jordan and Pauli, he expressed confidence in the method to quantize the electromagnetic and the electron wave. Then he continued (curly brackets  $\{ \dots \}$  denote passages which were omitted in the second edition 1931 and the English translation, angular brackets  $\langle \dots \rangle$  an addition in the second edition):

We have thus discovered the correct way to quantize the field equations (...) defining light waves and electron waves {The exact execution is the next task of quantum physics. The preservation of relativistic invariance seems to offer serious difficulties [reference to Jordan/Pauli (1928) and Mie (1928), E.S.] }. Here again we find  $\langle$ , as in the case of the spinning electron, $\rangle$  that quantum kinematics is not to be restricted by the assumption of Heisenberg’s specialized commutation rules. {And again it is group theory which furnishes us with the natural general form, as is shown in the next section. ... } (Weyl, 1928, 1st ed. 1928, 203), (Weyl, 1931, 253)<sup>26</sup>

The “next section” of the first edition comprised the content of Weyl (1927).<sup>27</sup> Thus even at the time when he finished his book on *Gruppentheorie und Quantenmechanik* (GQM), Weyl apparently had the impression that the study of irreducible ray representations and a group theoretically founded approach to quantization ought to be helpful for a full solution of the “dynamical problem” of quantum physics, i.e., the study of interactions and for relativistic systems. His colleagues in physics started to attack such problems by introducing the method of field quantization.

By the early 1930s Weyl became more cautious. His physics colleagues had embarked even more strongly on the program of field quantization, including the relativistic case. The great problems of divergent field expressions, even for perturbation developments, were accumulating. Weyl did no longer try to pursue his own approach against the mainstream of the (still very small) quantum physics community; he may have felt that he should no longer insist on the superiority of the group approach to the foundations

<sup>26</sup>“Damit ist der Weg gezeigt, wie die Licht- und Elektronenwellen umfassenden Feldgleichungen in richtiger Weise zu quantisieren sind. {Die genaue Durchführung ist die nächste Aufgabe der Quantenphysik; die Wahrung der relativistischen Invarianz scheint dabei noch ernste Schwierigkeiten zu bereiten. [Verweis auf Jordan/Pauli (1928) and Mie (1928), E.S.]} Es hat sich hier von neuem  $\langle$ , wie beim Spin der Elektronen, $\rangle$  die Notwendigkeit herausgestellt, die Quantenkinematik nicht an das spezielle Schema der Heisenbergschen Vertauschungsrelationen zu binden.” Robertson’s translation of the first sentence in Weyl (1931) has been corrected by obvious reasons (“... electron waves and matter waves ...” is non-sensical and not in agreement with the original).

<sup>27</sup>In the second edition and in the English translation new sections on the quantization of the Maxwell-Dirac field and on relativistic invariance were inserted before the section on quantum kinematics (Weyl, 1931, §§ 12, 13).

of quantum physics, if he himself did no longer continue to work along these lines.<sup>28</sup> In the second edition of GQM, and thus in the English translation, the (curly) bracketed sentences no longer appeared.

Notwithstanding this shift at the turn to the 1930s, Weyl had good reasons in the late 1920s to be content with his group theoretic approach to the foundations of QM. He had arrived at a convincing structural characterization of what he called the “quantum kinematics” of physical systems. For  $n$  continuous degrees of freedom, the quantum kinematics was even uniquely determined by  $n$ . Not so, however, for discrete systems in which the noncommutative product structure of the algebra of observables might become more involved. Weyl indicated very cautiously that such structures might perhaps be useful for the understanding of atomic systems; but he was far from claiming so (Weyl, 1928, 207) (Weyl, 1931, 276).

## Outlook and Repercussions

Weyl’s approach to quantization was so general that for decades to come it did not attract much attention of physicists. At the beginning it even attracted very few successor investigations inside mathematics and was not noticed in the foundation of QM discourse, which was exclusively shaped by the Hilbert and von Neumann view until the 1950s. Although the immediate reception of Weyl’s early contributions to QM until about 1927, in particular his Weyl (1927), was very sparse, its repercussion turned out to be *remarkably strong in the long range*. Of course, this question touches a difficult matter and deserves much closer and more detailed scrutiny. Here I can give only a very rough first outline. It will be given in form of a provisional list of investigations which seem to count as follow up stories to the proposals made by Weyl between 1925 and 1927.

- (i) A first and immediate next step was made by *Marshall Stone* and *John von Neumann*. They both took up Weyl’s statement of a uniquely determined structure of irreducible unitary ray representations of  $\mathbb{R}^{2n}$  and proved it for  $n = 1$  in  $\mathcal{L}^2(\mathbb{R}, \mathbb{C})$ . The result of this work is (for finite  $n$ ) the now famous *Stone/von Neumann representation theorem*: Up to isomorphism there is exactly one irreducible abelian ray representation of  $\mathbb{R}^{2n}$  by unitary operators Stone (1930); von Neumann (1931). As we have seen its content and a sketch of proof, generously passing over the functional analytical details in silence, goes back to Weyl (1927).

Only much later a critical analysis of functional analytic preconditions for the equivalence of Heisenberg commutation (13.9) and Weyl commutation (13.10) started. Sufficient conditions were established by Friedrich (1946) and Dixmier. The breakdown of uniqueness for infinite degrees of freedom (and thus for quantum field theory) started with seminal work by Kurt Friedrichs and Rudolf Haag in the 1950s. Construction of “pathological” counter-examples, disregarding the conditions of Rellich and Dixmier, even for the finite dimensional case ( $n = 1$ ) followed Summers (2001).

---

<sup>28</sup>The non-uniqueness problem for irreducible unitary representations of infinite dimensional degrees of freedom, and thus for quantum field theory, was realized only in the 1950s Summers (2001); it seems unlikely that Weyl expected a problem in this respect already at the turn to the 1930s.

- (ii) A second line of repercussions may be seen in that part of the work of *E. Wigner* and *V. Bargmann*, which dealt with unitary and *semi-unitary ray representations*. In particular Wigner's now famous work (at the time among physicists completely neglected) on the *irreducible unitary ray representations of the Poincaré group* Wigner (1939) looks like a next step beyond Weyl's non-relativistic quantum kinematics from 1927. It established a basis from which investigations of relativistic dynamics might start from. But it has still to be checked in which respect, or perhaps even whether, Wigner was motivated by Weyl's work. Wigner surely knew the latter, but he may have developed his research questions autonomously, in communication with von Neumann, Dirac and others which stood closer to him than Weyl.<sup>29</sup>
  
- (iii) A third impact is clearly to be seen in *George Mackey's* work. Mackey expressly took up Weyl's perspective Mackey (1949) and developed it into a broader program for the study of *irreducible unitary representations of group extensions*,  $H \triangleleft G$ , induced from representations of a normal subgroup  $H$  in  $G$ , by what he called *systems of imprimitivity*. Starting at first from abelian subgroups  $H$ , he realized that the dual group  $\hat{H}$  led to a pairing characteristic for Weyl's analysis ( $H \cong \mathbb{R}^n, H \times \hat{H} \cong \mathbb{R}^{2n}$ ) and generalized it to non-abelian normal subgroups. His later commentaries on the *foundations of QM*, among them Mackey (1957, 1963, 1993), were seminal for bringing to bear the Weylian perspective in the domain of foundations of quantum physics. They were so deeply influenced by the Weylian view, that Mackey even considered his work as the true successor line of Weyl's foundational perspective Mackey (1988*b,a*). His work was influential among mathematicians Varadarajan (1970), although apparently not so much among physicists. It seems to contain unexhausted potential.
  
- (iv) Finally, *Weyl quantization* was taken up by mathematical physicists from the later 1960s onwards with the rise of *deformation quantization* Pool (1966). Here the starting point was the idea to translate the operator product introduced by Weyl's own quantization

$$f, g \rightarrow H := \mathcal{F}(f) \circ \mathcal{F}(g)$$

back to the function space:

$$f * g =: h \iff \mathcal{F}(h) = H = \mathcal{F}(f) \circ \mathcal{F}(g)$$

Today, this noncommutative product of functions is usually considered (slightly anachronistically) as *Weyl quantization*. Weyl's mixed continuous-discrete group (13.15) developed into the noncommutative torus. This was one step into the newly rising field of noncommutative geometry and deformation quantization, which is a very active subfield of present day mathematical physics.

---

<sup>29</sup>Wigner expressly acknowledged the importance of Dirac's and von Neumann's communications for his work (Wigner, 1939, 341/156); whereas he quoted Weyl only in questions of technical details and Weyl (1927) not at all. On the other hand, Mackey is certainly right in the characterization of Wigner (1939): "This kind of application of the theory of group representations to quantum mechanics is much more in the spirit of Weyl's 1927 paper in the *Zeitschrift für Physik* than that of most of Wigner's work up to this point" (? , 265).

The last two points lead straight into very recent developments of mathematical physics and far beyond the scope of this talk (and my competences). Nevertheless it seems quite remarkable that at least two of Weyl's ideas developed in the first two years after the transition to the 'new' quantum mechanics, turned out to bear fruits in so diverse directions in the long run. They inspired highly original work for more than half a century and perhaps contain the potential to continue to do so.

Both ideas happen to have been mentioned at the very beginning of this phase in Weyl's correspondence with Born and Jordan, in late summer and autumn 1925. In this correspondence Weyl contributed to the new quantum physics discourse in a more personal form, before he turned toward published expression of his views two years later.

## Bibliography

- Bochner, Solomon. 1927. "Darstellung reell variabler und analytischer Funktionen durch verallgemeinerte Fourier- und Laplaceintegrale." *Mathematische Annalen* 97:635ff.
- Born, Max. 1963. *Ausgewählte Abhandlungen*. Göttingen: Vandenhoeck und Ruprecht.
- Born, Max. Ms 1925. "Letter to H. Weyl, October 2, 1925." Nachlass Weyl, ETH Zürich, Hs 91:488.
- Born, Max; Jordan, Pascual. 1925. "Zur Quantenmechanik." *Zeitschrift für Physik* 34:858–888. (Received September 27, 1925, published November 28, 1925.) In (Born, 1963, II, 124–154).
- Deppert, W. e.a. (ed.s.). 1988. *Exact Sciences and Their Philosophical Foundations*. Frankfurt/Main: Peter Lang. Weyl, Kiel Kongress 1985.
- Friedrich, Rellichm. 1946. "Der Eindeutigkeitssatz für die Lösungen der quantenmechanischen Vertauschungsrelationen." *Nachrichten Akademie der Wissenschaften Göttingen, Math-Phys. Klasse* 11 A:107–115.
- Hardy, Godfrey H.; Littlewood, John E. 1926. "Note on two theorems of N. Wiener." *Journal London Mathematical Society* 1:240–245. In: Hardy, G. H. *Collected Papers*, VII, 139–244.
- Hawkins, Thomas. 2000. *Emergence of the Theory of Lie Groups. An Essay in the History of Mathematics 1869–1926*. Berlin etc.: Springer.
- Jordan, Pascual. 1927. "Über eine neue Begründung de Quantenmechanik." *Zeitschrift für Physik* 40:809–838.
- Jordan, Pascual. Ms 1925. "Letter to H. Weyl, November 25, 1925." Nachlass Weyl, ETH Zürich, Hs 91:626.
- Jordan, Pascual; Pauli, Wolfgang. 1928. "Zur Quantenelektrodynamik ladungsfreier Felder." *Zeitschrift für Physik* 43:151–173. In: Pauli, W. *Collected Scientific Papers*, II, 331–353.
- Mackey, George. 1949. "Imprimitivity for representations of locally compact groups." *Proceedings National Academy of Sciences USA* 35:537–544.
- Mackey, George. 1957. "Quantum mechanics and Hilbert space." *American Mathematics Monthly* 64:45–57.
- Mackey, George. 1963. *Mathematical Foundations of Quantum Mechanics*. New York: Benjamin.

- Mackey, George. 1988*a*. “Hermann Weyl and the application of group theory to quantum mechanics.”. In (Deppert, 1988, 131–160).
- Mackey, George. 1988*b*. Weyl’s program and modern physics. In *Differential Geometric Methods in Theoretical Physics*, ed. K. Bleuler; M. Werner. Dordrecht: Kluwer pp. 11–36. Reprint in (Mackey, 1992, 249–274).
- Mackey, George. 1992. *The Scope and History of Commutative and Noncommutative Harmonic Analysis*. Providence, Rhode Island: AMS.
- Mackey, George. 1993. “Axiomatics of particle interaction.” *International Journal for Theoretical Physics* 32:1743–1659.
- Mie, Gustav. 1928. “Untersuchungen zum Problem der Quantenelektrik.” *Annalen der Physik* 390:711–729.
- Pool, J.C.T. 1966. “Mathematical aspects of the Weyl correspondence.” *Journal for Mathematical Physics* 7:66–76.
- Rédei, Miklóš; Stöltzner, Michael (eds.). 2001. *John von Neumann and the Foundations of Quantum Mechanics*. Dordrecht etc.: Kluwer.
- Scholz, Erhard. 2004*a*. The changing concept of matter in H. Weyl’s thought, 1918–1930. In *The interaction between Mathematics, Physics and Philosophy from 1850 to 1940*, ed. J. Lützen. Dordrecht etc.: Kluwer. [<http://arxiv.org/math.HO/0409576>].
- Scholz, Erhard. 2004*b*. “Hermann Weyl’s analysis of the “problem of space” and the origin of gauge structures.” *Science in Context* 17:165–197.
- Scholz, Erhard. 2005. Local spinor structures in V. Fock’s and H. Weyl’s work on the Dirac equation (1929). In *Géométrie au XXIème siècle, 1930 – 2000. Histoire et Horzions*, ed. D. Flament; J. Kounieher; P. Nabonnand; J.-J. Szczeciniarz. Paris: Hermann pp. 284–301. [<http://arxiv.org/physics/0409158>].
- Scholz, Erhard. 2006. “Introducing groups into quantum theory (1926–1930).” *Historia Mathematica* 33:440–490. [<http://arxiv.org/math.HO/0409571>].
- Schrödinger, Erwin. 1926. “Abhandlungen zur Wellenmechanik.” *Annalen der Physik* 81:133. Reprint Leipzig 1927, 163ff. In (Schrödinger, 1984, vol. 3).
- Schrödinger, Erwin. 1984. *Gesammelte Abhandlungen*, 4 Bde.. Wien: Österreichische Akademie der Wissenschaften.
- Stone, Marshall. 1930. “Linear operators in Hilbert space.” *Proceedings National Academy of Sciences USA* 16:172–175.
- Summers, Stephen J. 2001. “On the Sone – von Neumann uniqueness theorem and its ramifications.”. In (Rédei, 2001, 135–152).
- von Neumann, Johann (János, John). 1931. “Die Eindeutigkeit der Schrödingerschen Operatoren.” *Mathematische Annalen* 104:570–578. In (von Neumann, 1961/1976, II, 221–229).

## Weyl Entering the 'New' Quantum Mechanics Discourse

---

- von Neumann, John (János, Johann). 1961/1976. *Collected Works*, 6 volumes, ed. A.H. Taub. Oxford etc.: Pergamon.
- Varadarajan, V.S.. 1970. *Geometry of Quantum Theory*, 2 vols. New York etc.: Van Nostrand. 2nd edition in one volume, Berlin etc.: Springer 1985.
- Weyl, Hermann. 1925/1926. "Theorie der Darstellung kontinuierlicher halbeinfacher Gruppen durch lineare Transformationen. I, II, III und Nachtrag." *Mathematische Zeitschrift* pp. 23 271–309, 24 328–395, 789–791. In (Weyl, 1968, II, 542–646) [68].
- Weyl, Hermann. 1927. "Quantenmechanik und Gruppentheorie." *Zeitschrift für Physik* 46:1–46. In (Weyl, 1968, III, 90–135) [75].
- Weyl, Hermann. 1928. *Gruppentheorie und Quantenmechanik*. Leipzig: Hirzel. <sup>2</sup>1931.
- Weyl, Hermann. 1931. *The Theory of Groups and Quantum Mechanics*. Translated from the 2nd German edition by H.P. Robertson. New York: Dutton.
- Weyl, Hermann. 1968. *Gesammelte Abhandlungen, 4 vols*. Ed. K. Chandrasekharan. Berlin etc.: Springer.
- Weyl, Hermann. Ms 1925a. "Letter to M. Born, September 27, 1925." Staatsbibliothek Berlin, Nachlass Jordan 965.
- Weyl, Hermann. Ms 1925b. "Letter to P. Jordan, November 13, 1925." Staatsbibliothek Berlin, Nachlass Jordan 638.
- Weyl, Hermann. Ms 1925c. "Postcard to P. Jordan, November 23, 1925." Staatsbibliothek Berlin, Nachlass Jordan 638.
- Wiener, Norbert. 1926. "On representations of functions by trigonometric integrals." *Mathematische Zeitschrift* 24:575–616.
- Wiener, Norbert. 1976–1985. *Collected Works with Commentaries*, 4 vols. Cambridge, Mass.: MIT Press.
- Wigner, Eugene. 1939. "On unitary representations of the inhomogeneous Lorentz group." *Annals of Mathematics* 40:149–204. In (Wigner, 1992ff., I, 334–389).
- Wigner, Eugene. 1992ff. *Collected Works*. Part A: The Scientific Papers, Part B: Historical, Philosophical, and Socio-Political Papers. Berlin etc.: Springer.





# 14 The Statistical Interpretation According to Born and Heisenberg

GUIDO BACCIAGALUPPI

*At the 1927 Solvay conference Born and Heisenberg presented a joint report on quantum mechanics. I suggest that the significance of this report lies in that it contains a ‘final’ formulation of the statistical interpretation of quantum mechanics that goes beyond Born’s original proposal. In particular, this formulation imports elements from Heisenberg’s work as well as from the transformation theory of Dirac and Jordan. I suggest further a reading of Born and Heisenberg’s position in which the wave function is an effective notion. This can make sense of a remarkable aspect of their presentation, namely the fact that the ‘quantum mechanics’ of Born and Heisenberg apparently lacks wave function collapse.*

## 14.1 Introduction

The fifth Solvay conference of 1927 saw the presentation of (and confrontation between) three fundamental approaches to quantum theory: de Broglie’s pilot-wave theory, Schrödinger’s wave mechanics, and ‘quantum mechanics’ (i.e. matrix mechanics and its further developments), the latter presented to the conference in a joint report by Born and Heisenberg.

A thorough examination of the conference proceedings reveals substantial amounts of material that are either little known or generally misrepresented. Such an examination is given in a forthcoming book on the 1927 Solvay conference (Bacciagaluppi and Valentini, 2008), which also includes a complete English version of the proceedings, based on the original-language materials where available.<sup>1</sup>

In this paper, I wish to focus on the report by Born and Heisenberg, arguing that it contains a version of the statistical interpretation of quantum mechanics that goes well beyond that elaborated by Born in his papers on collisions and in his paper on the adiabatic theorem (Born, 1926a,b,c). In particular, the report offers an interpretation of the interference of probabilities, which appears to be related to Heisenberg’s ideas as developed in his uncertainty paper (Heisenberg, 1927).

I shall further propose a reading of Born and Heisenberg’s position in which the wave function has no fundamental status, in a way related to Heisenberg’s paper on fluctuations (Heisenberg, 1926). Born and Heisenberg’s report should thus indeed be seen as presenting an approach that is fundamentally different from both de Broglie’s pilot-wave theory and Schrödinger’s wave mechanics.

---

<sup>1</sup>Quotations below from the proceedings of the conference are based on this English edition; page references are to the corresponding passages of the on-line draft available at <http://xxx.arxiv.org/abs/quant-ph/0609184>.

Finally, I suggest that the proposed reading makes sense of an aspect of Born and Heisenberg's presentation (and of the discussions) that is especially puzzling from the point of view of a modern reader, namely the almost total absence of the 'collapse of the wave function' or 'reduction of the wave packet'.

Much of the material presented below is based on Bacciagaluppi and Valentini (2008),<sup>2</sup> including parts of the book that are joint work or even principally the work of my coauthor (the latter especially in section 14.3). However, the perspectives on this material adopted in the paper and in the book are very different. The idea of a 'definitive' version of the statistical interpretation merging elements from Born's and Heisenberg's work is hardly mentioned in the book. Furthermore, the presentation in the book is uncommittal about the views on collapse and on the status of the wave function held by Born and Heisenberg. This paper instead attempts to put forward one particular reading (not because it is unequivocally supported by the evidence, but as a proposal for making sense of the material that will need further evaluation).

It is useful therefore to spell out at least some of the differences between the treatment of the material in this paper and in Bacciagaluppi and Valentini (2008). First of all, as emphasised already, here I suggest that the report is a new stage of development of the statistical interpretation. This is something that is left largely implicit in the discussion in the book. Here I suggest that Born and Heisenberg present a single coherent position. The treatment in the book allows for possible differences in opinion between the two authors (emphasising for instance the possible relation between Born's discussion of the cloud chamber and the guiding-field ideas in his collision papers). Here I try to make explicit links between Born and Heisenberg's implicit notion of state in their treatment of transition probabilities on the one hand, and Born's treatment of the cloud chamber on the other; I also hint at the possibility that Pauli had such a link in mind. Neither suggestion is made in the book. Last but not least, I suggest here that Born and Heisenberg did not believe in the reality of the wave function. This is mentioned in the book only as one tentative possibility among others.

Bacciagaluppi and Valentini (2008) refrains on purpose from drawing conclusions from the material that might have been premature. This paper hopes to be a first step in drawing further conclusions. Indeed, while the interpretation of quantum theory seems as highly controversial again today as it was in 1927, from the vantage point of eighty years of philosophy of quantum physics a more dispassionate evaluation of the sources in the interpretation debate should be possible. I wish to thank Antony Valentini for discussion and comments during the preparation of this paper, although of course all deviations from and additions to the presentation of the material as given in the book are my sole responsibility.

---

<sup>2</sup>The report itself and the discussion following it are translated and annotated on pp. 408–447. Born and Heisenberg's views are analysed and discussed principally in chapters 3 and 6. Among the topics discussed in this paper, the main ones treated in the book are the following. Born and Heisenberg's treatment of interference is discussed in section 6.1.2 (pp. 172–177). The derivation of transition probabilities in Born's collision papers and in Heisenberg's fluctuations paper are discussed, respectively, in section 3.4.3 (pp. 107–108) and 3.4.4 (pp. 109–111). Phase randomisation in measurement is discussed in detail on pp. 173–177. Extensive presentations and analyses of Born's discussion of the cloud chamber and of the exchange between Heisenberg and Dirac are given, respectively, in sections 6.2 (pp. 177–182) and 6.3 (pp. 182–189). Finally, Einstein's alternative hidden-variables proposal (with Heisenberg's comments) is discussed in detail in section 11.3 (pp. 259–265).

## 14.2 The Statistical Interpretation in Born and Heisenberg's Report

The report by Born and Heisenberg on 'quantum mechanics' is surprisingly difficult for the modern reader. This is partly because Born and Heisenberg are describing various stages of development of the theory that are quite different from today's quantum mechanics. At the same time, the interpretation of the theory also appears to have undergone important modifications, in particular regarding the notion of the state of a system (see Bacciagaluppi and Valentini, 2008, section 3.4).

It is known which sections of the report were drafted by Born and which by Heisenberg. In particular, the section most relevant to our concerns—that on the 'Physical interpretation' of the theory—was drafted by Born, who also prepared the final version of the paper, although Heisenberg made some further small changes.<sup>3</sup> As we shall see, the interpretation presented merges crucially elements of Born's and Heisenberg's work, and (at least for the purposes of this paper) we shall consider the interpretational views as set forth in the report (and in the discussions reported below) as expressing a common voice. This is also supported by Born's remark to Lorentz that Heisenberg and he were 'of one and the same opinion on all essential questions'.<sup>4</sup>

### 14.2.1 The Statistical Interpretation

Until the 1927 report, the most explicit presentation of the statistical interpretation of quantum theory was that given in Born's paper on the adiabatic theorem (1926c). The picture presented by Born is as follows. Particles exist, at least during periods in which systems evolve freely (say, between 0 and  $t$ ). At the same time, they are accompanied by de Broglie-Schrödinger waves  $\psi$ . Regardless of the form of these waves, during a period of free evolution a system is always in a stationary state. When the waves  $\psi$  are developed in the basis of eigenstates  $\psi_n(x)$  of energy, say

$$\psi(x, 0) = \sum_n c_n \psi_n(x) , \quad (14.1)$$

they yield the probabilities for the occurrence of the stationary states, the 'state probabilities' being given by  $|c_n|^2$ . During periods, say from  $t$  to  $T$ , in which an external force is applied (or the system interacts with another system) there may be no anschaulich representation of the processes taking place. As regards the particles, the only thing that can be said is that 'quantum jumps' occur, in that after the external influence has ceased the system is generally in a different stationary state. The evolution of the state probabilities instead is well-defined and determined by the Schrödinger equation, in the sense that the state probabilities at time  $T$  are given by the corresponding expression  $|C_n|^2$  of the coefficients of  $\psi(x, T)$ .

For the case in which  $\psi(x, 0) = \psi_n(x)$ , Born determines explicitly these coefficients, call them  $b_{nm}$ , in terms of the time-dependent external potential; thus,

$$\psi(x, T) = \sum_m b_{nm} \psi_m(x) . \quad (14.2)$$

<sup>3</sup>Born to Lorentz, 29 August 1927, AHQP-LTZ-11 (in German). Cf. Bacciagaluppi and Valentini (2008, section 3.2).

<sup>4</sup>Born to Lorentz, *loc. cit.*; quoted with the kind permission of Prof. Gustav Born.

Given the interpretation of the quantities  $|b_{nm}|^2$  as state probabilities, in this case they are also the ‘transition probabilities’ for the jump from the initial state, which by assumption is  $\psi_n(x)$  at time  $t$ , to the final state  $\psi_m(x)$  at time  $T$ .

Finally, for the general case of an initial superposition (14.1), Born states that the state probabilities  $|C_n|^2$  have the form

$$|C_n|^2 = \left| \sum_m c_m b_{mn} \right|^2, \quad (14.3)$$

noting that (1926c, p. 174):

The quantum jumps between two states labelled by  $m$  and  $n$  thus do *not* occur as independent events; for in that case the above expression should be simply  $\sum_m |c_m|^2 |b_{mn}|^2$

(with a footnote to Dirac (1926) as also pointing out this fact<sup>5</sup>). He also remarks that, as he will show later on, the quantum jumps become independent in the case of an external perturbation by “natural” light’.

As it appears in Born’s adiabatic paper, the statistical interpretation is quite different both from the familiar textbook interpretations and from the interpretation we shall find in Born and Heisenberg’s Solvay report. For instance, the requirement that the state of an isolated system be always a stationary state is unfamiliar, to say the least. (As we shall see, it is eventually relaxed in Born and Heisenberg’s report.)

For now let us focus on Born’s remark about quantum jumps not being independent. This terminology appears to presuppose a probability space in which the elementary events do not correspond to single systems performing quantum jumps, but to  $N$ -tuples of systems all performing quantum jumps between  $t$  and  $T$ .<sup>6</sup> (The analogous case in classical statistical mechanics is the treatment of gases of interacting rather than non-interacting particles.)

If this is the correct way of understanding Born’s statistical interpretation of the wave function (at least as proposed in 1926), then Einstein may well have had Born’s view in mind when at the 1927 Solvay conference he criticised what he labelled ‘conception I’ of the wave function (p. 487):<sup>7</sup>

The de Broglie-Schrödinger waves do not correspond to a single electron, but to a cloud of electrons extended in space. The theory gives no information about individual processes, but only about the ensemble of an infinity of elementary processes.

According to Einstein, it is only the alternative ‘conception II’, in which the wave function is a complete description of an individual system (and which he also goes on to criticise), that enables one to derive the conservation laws, the results of the Bothe-Geiger experiments and the straight tracks of  $\alpha$ -particles in a cloud chamber. Note that the last example is taken up by Born in the general discussion (see below section 14.3.2).

---

<sup>5</sup>Cf. especially pp. 674 and 677 of Dirac’s paper.

<sup>6</sup>Born’s discussion of natural light later in the paper only reinforces this impression. Born assumes that due to the irregular temporal course of the external perturbation, the  $b_{nm}$  will fluctuate independently.

<sup>7</sup>For an alternative interpretation of Einstein’s comments, see Bacciagaluppi and Valentini (2008, p. 225).

Be it as it may, Born's paper on the adiabatic theorem lacks a separate discussion of interference; and this is the crucial point where the report by Born and Heisenberg goes further than Born's paper. Born and Heisenberg (p. 423) consider an atom that is initially in a superposition of energy states  $\psi_n(x)$ , with coefficients  $c_n(0) = |c_n(0)| e^{i\gamma_n}$  and eigenvalues  $E_n$ . The Schrödinger equation induces a time evolution

$$c_n(t) = \sum_m S_{nm}(t) c_m(0) . \quad (14.4)$$

In the special case where  $c_m(0) = \delta_{mk}$  for some  $k$ , we have  $|c_n(t)|^2 = |S_{nk}(t)|^2$ , and Born and Heisenberg interpret  $|S_{nk}(t)|^2$  as a transition probability. They also draw the conclusion that 'the  $|c_n(t)|^2$  must be the state probabilities' (p. 424). Thus far the discussion is reminiscent of Born's treatment, and Born and Heisenberg in fact quote Born's paper on the adiabatic principle in support of this interpretation.

At this point, however, Born and Heisenberg recognise a 'difficulty of principle' (p. 424), which is precisely that for an initial superposition of energy states the final probability distribution is given by

$$|c_n(t)|^2 = \left| \sum_m S_{nm}(t) c_m(0) \right|^2 , \quad (14.5)$$

as opposed to

$$|c_n(t)|^2 = \sum_m |S_{nm}(t)|^2 |c_m(0)|^2 . \quad (14.6)$$

This 'theorem of the interference of probabilities' in Born and Heisenberg's words appears to contradict what 'one might suppose from the usual probability calculus' (p. 424).

Born and Heisenberg then make a remarkable statement (pp. 424–425):

.... it should be noted that this 'interference' does not represent a contradiction with the rules of the probability calculus, that is, with the assumption that the  $|S_{nk}|^2$  are quite usual probabilities. In fact, .... [(14.6)] follows from the concept of probability .... when and only when the relative number, that is, the probability  $|c_n|^2$  of the atoms in the state  $n$ , has been *established* beforehand *experimentally*. In this case the phases  $\gamma_n$  are unknown in principle, so that [(14.5)] then naturally goes over to [(14.6)] .... .

We shall return in the next section to Born and Heisenberg's characterisation of the role of the experiment. What they are saying about the probability calculus is that the expressions  $|S_{nk}|^2$  denote 'usual' transition probabilities *irrespective* of whether they appear in (14.5) or in (14.6). Instead, the reason for the failure of (14.6) to hold in general is that the expressions  $|c_m|^2$  are not always state probabilities, because the state probabilities themselves are not always well-defined (Bacciagaluppi and Valentini, 2008, pp. 175–176). If the state probabilities are well-defined (namely if the energy has been measured, in general non-selectively), then one can calculate them at future times using (14.6). The truth of this conditional statement, however, is not affected if the state probabilities in fact are not always well-defined.

This, now, is analogous to Heisenberg's famous discussion of the 'law of causality' in his uncertainty paper: the law is again a conditional statement, which remains true although the state of the system is defined in fact only to within the accuracy given by

the uncertainty principle. In Heisenberg's own words: '.... in the sharp formulation of the law of causality, "If we know the present exactly, we can calculate the future", it is not the consequent that is wrong, but the antecedent. We cannot in principle get to know the present in all determining data' (Heisenberg, 1927, p. 197).<sup>8</sup>

What Born and Heisenberg mean by 'usual' transition probabilities is evidently not the idea of conditional probabilities defined as quotients of the absolute probabilities, since for them the latter are not always well-defined. Instead they must mean some kind of potentialities, some probabilistic 'field of force', existing independently of the presence of a 'test particle'.

Regarding the 'state' of the system, the picture they have in mind seems to be similar to that in Born's papers: namely, that the actual state of the atom is a state of definite energy. The difference to the earlier picture is that now the stationary states exist or have a well-defined distribution only upon measurement (although the question of why this should be so is not explicitly addressed). Instead, the wave function merely defines a statistical distribution over the stationary states.

The step to considering arbitrary observables, and not just the energy, as having definite values only upon measurement is now very easy.<sup>9</sup> In order to extend the above picture to the general case, one has to generalise Born and Heisenberg's notion of transition probability to the case in which two different observables are measured at the beginning and the end of a given time interval. Here Born and Heisenberg are not very explicit. What they actually do in the report is to define 'relative state probabilities', i.e. equal-time conditional probabilities for values of one quantity given the value of another, in terms of the projections of the eigenvectors ('principal axes') of one quantity onto the eigenvectors of the other. (In modern terminology, it is of course these expressions that are called 'transition probabilities'.) In this they follow Dirac's (1927) and Jordan's (1927b,c) development of the transformation theory, which Heisenberg understood as generalising the ideas of his paper on fluctuations (Heisenberg, 1926).<sup>10</sup>

### 14.2.2 Transition Probabilities and the Status of the Wave Function

In Born's work as presented above, the statistical interpretation is an interpretation of Schrödinger's theory, albeit 'in Heisenberg's sense' (Born, 1926c, p. 168). As we shall see now, instead, Born and Heisenberg in the report do not start directly with the Schrödinger equation. I shall suggest that in Born and Heisenberg's view, although they may be very useful tools both for calculational purposes and for understanding interference, the wave function and the Schrödinger equation are only effective notions.

Section II of the report, on the 'physical interpretation' of quantum mechanics, begins with the following statement (p. 420):

The most noticeable defect of the original matrix mechanics consists in that at first it appears to give information not about actual phenomena, but

---

<sup>8</sup>On Heisenberg's treatment of the 'law of causality', see also Beller (1999, pp. 110–113).

<sup>9</sup>Again, Heisenberg's uncertainty paper (Heisenberg, 1927, pp. 190–191), as well as his correspondence with Pauli (Heisenberg to Pauli, 23 February 1927, in Pauli, 1979, pp. 376–382) both mention explicitly the loss of a privileged status for stationary states.

<sup>10</sup>Heisenberg to Pauli, 23 November 1926: 'Here [in Copenhagen] we have also been thinking more about the question of the meaning of the transformation function  $S$  and *Dirac* has achieved an extraordinarily broad generalisation of this assumption from my note on fluctuations' (in Pauli, 1979, p. 357).

rather only about possible states and processes. It allows one to calculate the possible stationary states of a system; further it makes a statement about the nature of the harmonic oscillation that can manifest itself as a light wave in a quantum jump. But it says nothing about when a given state is present, or when a change is to be expected. The reason for this is clear: matrix mechanics deals only with closed periodic systems, and in these there are indeed no changes. In order to have true processes, as long as one remains in the domain of matrix mechanics, one must direct one's attention to a *part* of the system; this is no longer closed and enters into interaction with the rest of the system. The question is what matrix mechanics can tell us about this.

As raised here, the question to be addressed is how to incorporate into matrix mechanics the (actual) state of a system, and the time development of such a state.

Two methods for introducing change into matrix mechanics are then presented. First of all, following Heisenberg's paper on fluctuation phenomena (Heisenberg, 1926), Born and Heisenberg consider the matrix mechanical description of two coupled systems in resonance. This they interpret in terms of quantum jumps between the energy levels of the two systems, and they give an explicit expression for the corresponding transition probabilities. It is only after this matrix mechanical discussion that Born and Heisenberg introduce the time-dependent Schrödinger equation as a way for describing time dependence. From this, Born and Heisenberg then derive transition probabilities following Born's adiabatic paper (1926c), as described above.

Already in the collision papers Born had aimed precisely at including into matrix mechanics a description of the transitions between stationary states (Born, 1926a,b). Born had managed to describe the asymptotic behaviour of the combined system of electron and atom solving by perturbation methods the time-independent Schrödinger equation, yielding a superposition of components associated to various, generally inelastic, collisions in which energy is conserved. Interpreting statistically the coefficients in the expansion, and since the incoming asymptotic wave function corresponds to a fully determined stationary state and 'uniform rectilinear motion',<sup>11</sup> one obtains the probabilities for quantum jumps from the given 'initial' state to the given 'final' state, i.e. the desired transition probabilities.<sup>12</sup>

At first Born may have thought that wave mechanical methods were indispensable for this purpose.<sup>13</sup> To Heisenberg's delight, however, Pauli was able to sketch how one could reinterpret Born's results in terms of matrix elements.<sup>14</sup> A few days later, Heisenberg

---

<sup>11</sup>This is, indeed, Born's terminology (1926a, p. 864; 1926b, p. 806). In this context, cf. also the discussion of Born and Wiener (1926) in Bacciagaluppi and Valentini (2008, section 3.4.1).

<sup>12</sup>Note that Born considers indeed two conceptually distinct objects: on the one hand the stationary states of the atom and the electron, on the other hand the wave function that defines the probability distribution over the stationary states. He reserves the word 'state' only for the stationary states.

<sup>13</sup>Cf. Born to Schrödinger, 16 May 1927: 'the simple possibility of treating with it aperiodic processes (collisions) made me first believe that your conception was superior' (quoted in Mehra and Rechenberg, 2000, p. 135).

<sup>14</sup>See Pauli to Heisenberg, 19 October 1926, in Pauli (1979, pp. 340–349), and Heisenberg's reply: 'Your calculations have given me again great hope, because they show that Born's somewhat dogmatic viewpoint of the probability waves is only one of many possible schemes' (Heisenberg to Pauli, 28 October 1926, in Pauli, 1979, p. 350).



sent Pauli the manuscript of his paper on fluctuation phenomena (Heisenberg, 1926), in which he developed considerations similar to Pauli's ones in the context of the example of two atoms in resonance. Indeed, starting from a closed system (thus stationary from the point of view of matrix mechanics) and focussing on the description of the subsystems, Heisenberg was able to derive explicit expressions for the transition probabilities within matrix mechanics proper, without having to introduce the wave function as an external aid. A very similar result was derived at the same time by Jordan (1927a), using two systems with a single energy difference in common.

Born's collision papers and the papers by Heisenberg and by Jordan can be all understood as seeking to obtain 'information ... about actual phenomena', by 'direct[ing] one's attention to a *part* of the system'. In this context, the fact that it is Heisenberg's setting rather than Born's which is chosen in the report suggests that Born and Heisenberg indeed intend to make the point that matrix mechanics can account for time-dependent phenomena without the aid of wave mechanics.

It is in this sense, I suggest, that one should read the following remark made by Born and Heisenberg between their introduction of the time-dependent Schrödinger equation and their discussion of transition probabilities and interference (p. 423):

Essentially, the introduction of time as a numerical variable reduces to thinking of the system under consideration as coupled to another one and neglecting the reaction on the latter, but this formalism is very convenient and leads to a further development of the statistical view.

In particular, I suggest that in Born and Heisenberg's view one should not simply interpret a time-dependent external potential in the Schrödinger equation (as used in the adiabatic paper for instance) as a substitute for the full Schrödinger equation of the combined system, but that the Schrödinger equation itself arises from considering only subsystems.<sup>15</sup>

This reading is further supported by Born and Heisenberg's remarks on generalising transition probabilities to the case of an arbitrary observable, which are now couched in terms that bypass wave functions entirely (pp. 428–429):

Alongside the concept of the relative state probability  $|\varphi(q', Q')|^2$ , there also occurs the concept of transition probability, namely, whenever one considers a system as depending on an external parameter, be it time or any property of a weakly coupled external system. Then the system of principal axes of any quantity becomes dependent on this parameter; it experiences a rotation, represented by an orthogonal transformation  $S(q', q'')$ , in which the parameter enters .... . The quantities  $|S(q', q'')|^2$  are the 'transition probabilities'; in general, however, they are not independent, instead the 'transition amplitudes' are composed according to the interference rule.

In part, reference to wave functions here is eliminated through a switch to the Heisenberg picture. One should note, however, that Born and Heisenberg manage to eliminate reference to the wave function completely *only* because they consider exclusively maximal observables. In the more general case of non-maximal (i.e. coarse-grained) observables,<sup>16</sup>

---

<sup>15</sup>Cf. also the derivation of time-dependent transition probabilities in Heisenberg (1930, pp. 148–150).

<sup>16</sup>And of course in the most general case of observables as positive-operator-valued measures (POVMs), for which see e.g. Peres (1993, pp. 282–289).

transition probabilities (whether in their sense or in the modern sense) depend also on the quantum state.

The overall picture one glimpses from these aspects of Born and Heisenberg's remarks is that what exists are just transition probabilities and measured values (although, as mentioned already, it is not explained why measurement should play such a special role).

As regards the transition probabilities, the  $|S_{nk}|^2$  defined by Born and Heisenberg are *independent* of the actual wave function. They can be calculated using the formalism of wave functions, namely as the coefficients in (14.4) for the case in which the initial wave function is the  $k$ th eigenstate of energy, but they are taken as the correct transition probabilities even when the initial wave function is arbitrary.

By way of contrast, one could take Bell's (1987) discrete and stochastic version of de Broglie's pilot-wave theory. In a theory of this type, given a choice of preferred observable ('beable' in Bell's terminology), the  $|c_n|^2$  are indeed always state probabilities, and one constructs appropriate transition probabilities that are generally different from Born and Heisenberg's  $|S_{nk}|^2$ , thereby explicitly retaining the validity of the standard formula (14.6). Evidently, Bell's transition probabilities must depend on the actual wave function of the system, which thus acts as a pilot wave, as in de Broglie's theory. Born and Heisenberg instead choose to give up the  $|c_n|^2$  as state probabilities and to keep the transition probabilities independent of the actual wave function (which is thus not a pilot wave in any sense).

In general, wave functions themselves can usefully represent statistical information about measured values, but one need not consider wave functions as describing the real state of the system (*contra* Schrödinger). In this sense, they appear to resemble more the Liouville distributions of classical mechanics, a comparison suggested also by some of Born and Heisenberg's remarks (p. 433):<sup>17</sup>

For some simple mechanical systems .... the quantum mechanical spreading of the wave packet agrees with the spreading of the system trajectories that would occur in the classical theory if the initial conditions were known only with the precision restriction [given by the uncertainty principle]. .... But in general the statistical laws of the spreading of a 'packet' for the classical and the quantum theory are different ....

As Darrigol (1992, p. 344) has emphasised, there is no notion of state vector either in Dirac's paper on the transformation theory (Dirac, 1927). (The well-known bras and kets do not appear yet.) The main result of Dirac's paper is to determine the conditional probability density for one observable given a value for a different observable, a result that Dirac illustrates by discussing precisely Heisenberg's example of transition probabilities in resonant atoms and Born's collision problem. As we shall see in section 14.3.3, however, by the time of the Solvay conference Dirac's and Born and Heisenberg's views had diverged, both with regard to whether the wave function should describe 'the state of the world', and with regard to the notion of the collapse of the wave function.

---

<sup>17</sup>Note also that in his discussion of the cloud chamber, Born once refers to the wave packet as a 'probability packet' (p. 483).

## 14.3 Measurements and Effective Collapse

It is remarkable that the reduction of the wave packet is totally absent from Born and Heisenberg's report, although this concept had been famously introduced by Heisenberg himself in the uncertainty paper (Heisenberg, 1927, p. 186). In this section we shall discuss what appears to take the place of reduction in Born and Heisenberg's report, then we shall focus on the two places in the conference proceedings where the reduction of the wave packet appears explicitly: Born's treatment of the cloud chamber in his main discussion contribution (pp. 483–486) and the intriguing exchange between Dirac and Heisenberg (pp. 494–497), both appearing in the general discussion at the end of the conference.

### 14.3.1 Measurement and Phase Randomisation

What is Born and Heisenberg's description of measurement? In the report, measurement appears only in the discussion of interference, namely, as we have seen, as the source for its suppression. This suppression of interference is achieved neither by applying the 'reduction of the wave packet' (i.e. not by collapsing the wave function onto the eigenstates of the measured observable) nor through entanglement of the measured system with the measuring apparatus (a simple form of what we would now call decoherence). The latter would in fact presuppose a quantum mechanical treatment of the interaction between the two, which was uncharacteristic for the time.

Instead, Born and Heisenberg appear to take measurement as introducing a randomisation of the phase in the wave function (Bacciagaluppi and Valentini, 2008, p. 173–177): indeed, they consider the case in which (p. 425):

.... the relative number, that is, the probability  $|c_n|^2$  of the atoms in the state  $n$ , has been *established* beforehand *experimentally*. In this case the phases  $\gamma_n$  are unknown in principle, so that [(14.5)] then naturally goes over to [(14.6)] ....

At this point Born and Heisenberg add a reference to Heisenberg's uncertainty paper, which indeed contains a more detailed version of essentially the same claim (see also below section 14.3.3). There, Heisenberg considers a Stern-Gerlach atomic beam passing through two successive regions of field inhomogeneous in the direction of the beam (so as to induce transitions between energy states without separating the beam into components). If the input beam is in a definite energy state then the beam emerging from the first region will be in a superposition. The probability distribution for energy emerging from the second region will then contain interference—as in (14.5), where the 'initial' superposition (14.1) is now the state emerging from the first region. Heisenberg asserts that, if the energy of an atom is actually measured between the two regions, then because of the resulting perturbation 'the "phase" of the atom changes by amounts that are in principle uncontrollable' (Heisenberg, 1927, pp. 183–184), and averaging over the unknown phases in the final superposition yields a non-interfering result.

This is clearly not the same as applying the collapse postulate. Indeed, if one applied the usual 'Dirac-von Neumann' postulate, after the measurement the atoms would be in eigenstates of energy, and the non-interfering result would be obtained by averaging over the different energy values.

The difference between the two descriptions is masked by the fact that the averages are the same, i.e. a statistical mixture of states of the superposed form (14.1), with randomly-distributed phases  $\gamma_n$ , is indeed statistically equivalent to a mixture of energy states  $\psi_n(x)$  with weights  $|c_n(0)|^2$ , because the corresponding density operators are the same. But for the subensembles selected on the basis of the measurement results (i.e. for the subensembles with definite values for the energy), the density operators are clearly different.

In the standard collapse case, indeed, the selected subensemble is homogeneous and described by a pure state  $\psi_n(x)$ . In the case of phase randomisation, taken literally, the subensembles selected on the basis of the measurement results are instead described by the *same* mixture of superposed states with randomly-distributed phases  $\gamma_n$ . If we take the state of the system (in the modern sense, i.e. the density operator) as determining the probabilities for the results of future measurements, we ought to conclude that in the case of phase randomisation an immediate repetition of the measurement will generally not yield the same result as the original measurement, and that any value could occur as a possible result.

However, if our reading above of Born and Heisenberg's discussion of the probability calculus is correct, the quantum state in the modern sense is *not* what determines the result of a subsequent measurement. While each atom in, say, the  $k$ th subensemble has a wave function of the form (14.1) with some unknown phases in the coefficients, we also know that it has the energy value  $E_k$ , because the energy has been measured and the atom has been selected precisely on the basis of this energy value. But now, according to Born and Heisenberg, the transition probabilities  $|S_{nk}|^2$  are independent of the actual wave function of the atom, so that if the atom is known to have the energy  $E_k$ , the statistical distribution of the energy values upon repetition of the measurement is simply given by (14.6) with  $c_m(0) = \delta_{mk}$ . If the repetition takes place immediately after the first measurement, the transition probabilities  $|S_{nk}|^2$  will tend to  $\delta_{nk}$ , so that indeed the first result will be confirmed (Bacciagaluppi and Valentini, 2008, p. 175–176).

One might dispute that the description of measurements as randomising the phases should be taken literally: it might be simply a rather sloppy way of talking about the decoherence induced by the measurement (encountered sometimes even today in discussions of decoherence in general).<sup>18</sup> However, the fact that Born and Heisenberg during the conference (and Heisenberg in the uncertainty paper) appear to use both the description of measurements in terms of phase randomisation and that in terms of reduction of the wave packet as equally good alternatives, may indicate that neither should be taken literally. The wave function can be chosen one way or another, depending on what is more convenient 'for practical purposes'.

### 14.3.2 Born's Discussion of the Cloud Chamber

In his discussion of the cloud chamber, Born attributes to Einstein the question of how one can account for the approximately straight particle track revealed by a cloud chamber, even if the emission of an  $\alpha$ -particle is undirected, so that the emitted wave

---

<sup>18</sup>My thanks to Antony Valentini for pointing out that a description of measurement in terms of phase randomisation appears also in Bohm's textbook on quantum mechanics (Bohm, 1951, pp. 122, 600–602).

function is approximately spherical.<sup>19</sup> Born asserts that to answer it (p. 483):

.... one must appeal to the notion of ‘reduction of the probability packet’ developed by Heisenberg. The description of the emission by a spherical wave is valid only for as long as one does not observe ionisation; as soon as such ionisation is shown by the appearance of cloud droplets, in order to describe what happens afterwards one must ‘reduce’ the wave packet in the immediate vicinity of the drops. One thus obtains a wave packet in the form of a ray, which corresponds to the corpuscular character of the phenomenon.

But then Born goes on to consider if wave packet reduction can be avoided by treating the atoms of the cloud chamber, along with the  $\alpha$ -particle, as a single system described by quantum theory, a suggestion that he attributes to Pauli. The latter had made this suggestion also in a letter to Bohr one week before the beginning of the Solvay conference:<sup>20</sup>

This is precisely a point that was not quite satisfactory in Heisenberg [(1927)]; there the ‘reduction of the packets’ seemed a little mystical. Now in fact it should be stressed that such reductions are not necessary in the first place if one includes *in* the system all means of measurement. But in order to describe at all observational results theoretically, one has to ask what one can say alone about a *part* of the whole system. And then from the complete solution one sees immediately that, in many cases (of course not always), leaving out the means of observation can be formally replaced by such reductions.

Born’s own opinion is as follows (p. 483):

Mr Pauli has asked me if it is not possible to describe the process without the reduction of wave packets, by resorting to a multi-dimensional space whose number of dimensions is three times the number of all the particles present .... . This is in fact possible and can even be represented in a very anschaulich manner [d’une manière fort intuitive] by means of an appropriate simplification, but this does not lead us further as regards the fundamental questions. Nevertheless, I should like to present this case here as an example of the multi-dimensional treatment of such problems.

Both Born and Pauli thus seem to think that the reduction of the wave packet is a dispensable element in the description of measurements.<sup>21</sup> However, Born’s subsequent discussion remains somewhat unclear about why this should be so. From the above quotation, it appears that the discussion is intended mainly as an illustration of the use of configuration-space wave functions (a point reiterated by Born at the end of his discussion). Born, indeed, merely presents a multi-dimensional treatment of the problem, simplified in that all motions are in one dimension and the cloud chamber is represented by only two atoms. Only in the end does Born remark that (p. 486):

---

<sup>19</sup>Cf. Einstein’s main contribution to the general discussion (pp. 486–488), and above, section 14.2.1.

<sup>20</sup>Pauli to Bohr, 17 October 1927, in Pauli (1979, p. 411).

<sup>21</sup>Note that also Pauli’s remarks to Heisenberg about transition probabilities and Born and Heisenberg’s treatment thereof, discussed in section 14.2.2, crucially make reference to ‘what one can say alone about a *part* of the whole system’. Pauli’s suggestion to Born and his remarks to Heisenberg may in fact be related.

To the ‘reduction’ of the wave packet corresponds the choice of one of the two directions of propagation  $+x_0$ ,  $-x_0$ , which one must take as soon as it is established that one of the two [atoms] 1 and 2 is hit ...

Now, provided this remark is at all relevant to the question of whether wave packet reduction is unnecessary, it should be read as an alternative to the description by means of reduction. That is, one should be able to leave the wave packet uncollapsed and choose *instead* a direction of propagation for the  $\alpha$ -particle, either because this is truly what happens upon measurement, or because the two descriptions are equivalent at least ‘for all practical purposes’, in which case presumably neither is to be taken literally.

Incidentally, the atoms in the cloud chamber are described by Born on the same footing as the  $\alpha$ -particle, making this perhaps the first example of explicit inclusion of a measuring apparatus in the quantum mechanical description. Note that the fact that the Schrödinger equation was not applied to the measurement interaction means that there was no awareness at the 1927 Solvay conference of the ‘measurement problem’, in the sense of macroscopic superpositions arising from the measurement interaction. For instance, also in Bohr’s famous exchanges with Einstein between the sessions of the conference (Bohr, 1949), Bohr applies only the uncertainty principle to the apparatus, and certainly not the Schrödinger equation, so that no macroscopic superpositions are considered. As regards Born’s example of the cloud chamber, it could have been used in principle to raise this problem. However, if the reading of Born and Heisenberg’s position suggested here is correct, it is not surprising that Born did not see the resulting macroscopic superposition as a problem, since the ‘state’ of the  $\alpha$ -particle (under the given conditions) would correspond indeed to its direction of motion.

### 14.3.3 The Exchange between Heisenberg and Dirac

Born’s remarks on the collapse of the wave function should be contrasted with Dirac’s remarks on the same topic, also in the general discussion (pp. 494–495):

According to quantum mechanics the state of the world at any time is describable by a wave function  $\psi$ , which normally varies according to a causal law, so that its initial value determines its value at any later time. It may however happen that at a certain time  $t_1$ ,  $\psi$  can be expanded in the form

$$\psi = \sum_n c_n \psi_n ,$$

where the  $\psi_n$ ’s are wave functions of such a nature that they cannot interfere with one another at any time subsequent to  $t_1$ . If such is the case, then the world at times later than  $t_1$  will be described not by  $\psi$  but by one of the  $\psi_n$ ’s. The particular  $\psi_n$  that it shall be must be regarded as chosen by nature.

This, according to Dirac (p. 495) is ‘an irrevocable choice of nature, which must affect the whole of the future course of events’. Dirac thus appears both to take the wave function to be a real physical object, and to take the collapse of the wave function to be a real physical process, connected with lack of interference (an interesting point both from today’s perspective and for the exchange with Heisenberg). But Dirac goes further, and recognises that there are circumstances where the choice made by nature

cannot have occurred at the point where it might have been expected. Dirac considers at some length the specific example of the scattering of an electron, concluding with the following observation (pp. 495–496):

If, now, one arranged a mirror to reflect the electron wave scattered in one direction  $d_1$  so as to make it interfere with the electron wave scattered in another direction  $d_2$ , one would not be able to distinguish between the case when the electron is scattered in the direction  $d_2$  and when it is scattered in the direction  $d_1$  and reflected back into  $d_2$ . One would then not be able to trace back the chain of causal events so far, and one would not be able to say that nature had chosen a direction as soon as the collision occurred, but only [that] at a later time nature chose where the electron should appear. The interference between the  $\psi_n$ 's compels nature to postpone her choice.

In Dirac's manuscript of this discussion contribution,<sup>22</sup> a cancelled version of the last sentence begins with 'Thus a possibility of interference ...', while another cancelled version begins with 'Thus the existence of interference ...'. Possibly, Dirac hesitated here because he saw that in principle the mirror could always be added by the experimenter after the scattering had taken place. Thus, there would be no cases in which interference could be ruled out as impossible, making this an unrealisable criterion for the occurrence of collapse.

Precisely this point was made by Heisenberg, shortly afterwards in the discussion (p. 497):

I do not agree with Mr Dirac when he says that, in the described experiment, nature makes a choice. Even if you place yourself very far away from your scattering material, and if you measure after a very long time, you are able to obtain interference by taking two mirrors. If nature had made a choice, it would be difficult to imagine how the interference is produced. I should rather say, as I did in my last paper [(Heisenberg, 1927)], that the *observer himself* makes the choice, because it is only at the moment when the observation is made that the 'choice' has become a physical reality and that the phase relationship in the waves, the power of interference, is destroyed.

Note the striking resemblance between what is said here by Heisenberg and what is said (more understatedly) by Born in his treatment of the cloud chamber. Born talks about the 'choice of one of the two directions of propagation', a choice which is taken not when one of the two atoms is hit, but when it is 'established' that it is hit (when the ionisation is 'shown' by the appearance of the cloud droplets); Heisenberg (who of course is also following Dirac's terminology) talks of a 'choice' of which path is taken by the electron, a choice which becomes physically real 'only at the moment when the observation is made'. But Heisenberg goes further than Born here, suggesting that what happens upon observation is that 'the phase relationship in the waves, the power of interference, is destroyed', i.e. that the effect of measurement is phase randomisation rather than collapse.

---

<sup>22</sup>AHQP-36, section 10.

## 14.4 Born and Heisenberg on ‘Hidden Variables’

To conclude, we shall now have a brief look at the views on what one would now call ‘hidden variables’ (in particular in the context of guiding fields) expressed at the time by Born and by Heisenberg, mostly before the Solvay conference. Indeed, the idea of observables having values that are not strictly linked to the wave function of the system (no ‘eigenstate-eigenvalue link’) might strike one as typical of hidden variables theories. This is precisely what happens in pilot-wave theories of the Bell type, as mentioned in section 14.3.1 above. Unsurprisingly, however, the views on the subject expressed by Born and by Heisenberg are quite negative.

### 14.4.1 Born on the Practical Irrelevance of Microcoordinates

Consider Born’s second paper on collisions (Born, 1926b). In this paper Born makes an explicit link between his work and guiding-field ideas, saying that while in the context of optics one ought to wait until the development of a proper quantum electrodynamics, in the context of the quantum mechanics of material particles the guiding field idea could be applied already, using the de Broglie-Schrödinger waves as guiding fields; these, however, determine the trajectories merely probabilistically (p. 804). In the concluding remarks of the paper, Born comments explicitly on whether this picture is to be regarded as fundamentally indeterministic (pp. 826–827):

In my preliminary communication [(Born, 1926a)] I laid very particular stress on this indeterminism, since it seems to me to correspond perfectly to the practice of the experimenter. But of course it is open to anyone who will not rest content therewith to assume that there are further parameters not yet introduced in the theory that determine an individual event. In classical mechanics these are the ‘phases’ of the motion, e.g. the coordinates of the particles at a certain instant. It seemed to me unlikely at first that one could freely include quantities in the new theory that correspond to these phases; but Mr Frenkel<sup>23</sup> has informed me that perhaps this in fact can be done. Be it as it may, this possibility would change nothing in the practical indeterminism of collision processes, since indeed one cannot give the values of the phases; it must lead, besides, to the same formulas as the ‘phaseless’ theory proposed here.

Thus, Born took it that a ‘completion’ of quantum mechanics through the introduction of further parameters into the theory would have no practical consequences, an opinion echoed in Born and Heisenberg’s report immediately after their introduction of transition probabilities (p. 422):

While the determinateness of an individual process is assumed by classical physics, practically in fact it plays no role, because the microcoordinates that determine exactly an atomic process can never all be given; therefore by averaging they are eliminated from the formulas, which thereby become

---

<sup>23</sup>This is presumably Y. I. Frenkel, who at the time was in Germany on a Rockefeller scholarship. Born had supported Frenkel’s application. (See Frenkel, 1996, p. 72).



statistical statements. It has become apparent that quantum mechanics represents a merging of mechanics and statistics, in which the unobservable microcoordinates are eliminated.

At the Solvay conference the idea of quantum mechanics as eliminating microscopic coordinates from the description of motions is mentioned by Born also in discussing Schrödinger's treatment of the Compton effect (p. 371; cf. also p. 444). It may have been an important element of Born's intuition, and appears also in Born's reaction to the EPR paper (Einstein, Podolsky and Rosen, 1935).<sup>24</sup>

#### 14.4.2 Heisenberg and Einstein on Hidden Variables

The above statements by Born may not rule out unequivocally the possibility of thinking of the wave function as a guiding field (more so perhaps his statements in the adiabatic paper on the Unanschaulichkeit of the quantum jump). Heisenberg's statements on the subject instead indicate both that he understood the principles behind pilot-wave theories and that he rejected them decidedly.

Heisenberg's views are contained in a letter to Einstein about the latter's own unpublished hidden-variables proposal (cf. Pais, 1982, p. 444). In May 1927, Einstein had proposed what in retrospect appears to be an alternative version of pilot-wave theory, with particle trajectories determined by the many-body wave function, but in a way different from that of de Broglie's theory. This theory was described in a paper entitled 'Does Schrödinger's wave mechanics determine the motion of a system completely or only in the sense of statistics?',<sup>25</sup> which was presented on 5 May 1927 at a meeting of the Prussian Academy of Sciences. On the same day Einstein wrote to Ehrenfest that '... in a completely unambiguous way, one can associate definite movements with the solutions [of the Schrödinger equation]' (quoted in Howard, 1990, p. 89). However, on 21 May, before the paper appeared in print, Einstein withdrew it from publication. The paper remained unpublished, but its contents are nevertheless known from the manuscript version in the Einstein archive—see also Belousek (1996) and Holland (2005).

Heisenberg had heard about Einstein's theory through Born and Jordan, and on 19 May—just two days before Einstein withdrew the paper—wrote to Einstein enquiring about it. On 10 June 1927, Heisenberg wrote to Einstein again, this time with detailed comments and arguments against what Einstein was (or had been) proposing. I shall now briefly summarise this second letter.<sup>26</sup>

Evidently, Einstein had not sent the withdrawn paper in reply to the original enquiry, for Heisenberg mentions he has learnt nothing new, but Heisenberg says he would like to write again why he believes indeterminism is '*necessary*, not just consistently possible'. If he has understood his viewpoint correctly, Einstein thinks that, while all experiments will agree with the statistical quantum theory, nevertheless in the future one will be able

---

<sup>24</sup>See Born to Schrödinger, 28 June 1935, AHQP-92, section 2 (in German).

<sup>25</sup>'Bestimmt Schrödingers Wellenmechanik die Bewegung des Systems vollständig oder nur im Sinne der Statistik?', Albert Einstein Archive 2-100.00; currently available on-line at <http://www.alberteinstein.info/db/ViewDetails.do?DocumentID=34338>.

<sup>26</sup>Heisenberg to Einstein, 19 May and 10 June 1927, Albert Einstein Archive 12-173.00 and 12-174.00 (both in German). Passages from the letter of 10 June are quoted with the kind permission of Prof. Helmut Rechenberg of the Werner Heisenberg Archive.

to talk also about definite particle trajectories. Heisenberg's main objection is now as follows.

Consider free electrons with a constant and low velocity, 'so slow, that the de Broglie wavelength is very large compared to the size of the particle, i.e. the force fields of the particle should be practically zero on distances of the order of the de Broglie wavelength'. Such electrons strike a grating with spacing comparable to their de Broglie wavelength. Heisenberg remarks that, in Einstein's theory, the electrons will be scattered in discrete spatial directions. Now, if the initial position of a particle were known one could calculate where the particle will hit the grating and 'set up some obstacle that reflects the particle in some *arbitrary* direction, quite independently of the other parts of the grating'. This could be done, if the forces between the particle and the obstacle act indeed only at short range, small with respect to the spacing of the grating. Heisenberg then continues:

In reality the electron is reflected independently of the obstacle in question in the definite discrete directions. One could only escape this if one sets the motion of the particle again in direct relation to the behaviour of the waves. But this means that one assumes that the size of the particle, that is, its interaction forces, depend on the velocity. Thereby one actually gives up the word 'particle' and loses in my opinion the understanding for why in the Schrödinger equation or in the matrix Hamiltonian function always appears the simple potential energy  $e^2/r$ . If you use the word 'particle' so liberally, I take it to be very well possible that one can define also particle trajectories. But the great simplicity that in the statistical quantum theory consists in that the motion of the particles takes place classically, insofar as one can talk of motion at all, in my opinion is lost.

Heisenberg then notes that Einstein seems willing to sacrifice this simplicity for the sake of maintaining causality. However, even Einstein's approach would not be able to change the fact that many experiments would be determined only statistically: 'Rather we could only console ourselves with the fact that, while for us because of the uncertainty relation  $p_1 q_1 \sim h$  the principle of causality would be meaningless, the good Lord in fact would know in addition the position of the particle and thereby could preserve the validity of the causal law'. Heisenberg concludes the objection by saying that he finds it 'actually not attractive [eigentlich doch nicht schön] to want to describe physically more than the connection between experiments'.

Note that Heisenberg's objection is not that the theory does not predict the usual scattering pattern in the practically unrealisable case in which one manipulates the trajectory of a particle with known initial position. Rather, his gedankenexperiment serves to establish the point that, even in the normal case (in which the initial position of the particle is unknown), the direction in which a 'particle' is scattered must depend only on the local features of the grating, thus contradicting the normal experimental results. The only way to have the direction of scattering depend on the features of the grating other than where the particle hits it, is to make the trajectory of the particle depend on the associated wave rather than on particle-like short-range interaction behaviour.

It is striking that Heisenberg's objection concerning the electron and the grating shows that he thought that a trajectory-based deterministic theory of quantum phenomena is possible. It is equally striking that Heisenberg appears to have thought that such a

theory is nevertheless unacceptable on what would seem to be aesthetic grounds (or grounds of *Anschaulichkeit*), because it gives up both the usual concept of particle and the mathematical simplicity of quantum mechanics. This objection appears to have remained a mainstay of Heisenberg's negative views on hidden variables. Indeed, Heisenberg repeated it also in his own draft reply to the EPR paper (Heisenberg, 1985, p. 416).<sup>27</sup>

## 14.5 Conclusion

In this paper, I have suggested that Born and Heisenberg's report at the 1927 Solvay conference is significant because it presents a more mature and definitive version of the statistical interpretation of quantum mechanics. The key point about this suggestion is that the interpretation in the report merges elements of Born's interpretational work of 1926 and of Heisenberg's work on fluctuations and in the uncertainty paper. I have also proposed a specific reading of Born and Heisenberg's position (thereby continuing where the analysis of Bacciagaluppi and Valentini, 2008, leaves off). The key intuition behind this proposal is that Born and Heisenberg did not take the wave function to be a real entity.

Of course, it is well-known that Heisenberg at least was strongly antagonistic to Schrödinger's introduction of wave functions and to his attempts to interpret them as giving an anschaulich picture of quantum systems. While Born's work of 1926 can be put in relation with ideas on guiding fields, I suggest that, at least come 1927, Born and Heisenberg's conception of the wave function was thoroughly statistical, i.e. more analogous to a classical Liouville distribution, thus making also the collapse of the wave function a matter of convenience of description. Born and Heisenberg's own words give the impression that they considered the presentation in their report to be indeed a final formulation of the theory and interpretation of quantum mechanics (pp. 409, 437):<sup>28</sup>

Quantum mechanics is meant as a theory that is in this sense anschaulich and complete for the micromechanical processes ([Heisenberg, 1927]) .... There seems thus to be no empirical argument against accepting fundamental indeterminism for the microcosm.

.... we consider [quantum mechanics] to be a closed theory [geschlossene Theorie], whose fundamental physical and mathematical assumptions are no longer susceptible of any modification.

Even as these views were being expressed, there remained significant differences of opinion even within the 'Göttingen-Copenhagen' camp (as seen in the exchange between Dirac and Heisenberg). Moreover, with its lack of collapse and perhaps even of fundamental wave functions, the interpretation presented was itself quite different from what might be assumed today to have been the 'statistical interpretation' of quantum theory.

---

<sup>27</sup>My thanks to Elise Crull for directing my attention to this passage in Heisenberg's draft.

<sup>28</sup>One can recognise Heisenberg's pen in these passages, which were in fact drafted by him (Born to Lorentz, *loc. cit.*, note 3). Cf. also Heisenberg's later writings on the concept of 'closed theories', e.g. Heisenberg (1948).

## References

- Bacciagaluppi, G., and Valentini, A. (2008), *Quantum Theory at the Crossroads: Reconsidering the 1927 Solvay Conference* (Cambridge: Cambridge University Press, forthcoming), arXiv:quant-ph/0609184v1.
- Bell, J. S. (1987), ‘Beables for quantum field theory’, in *Speakable and Unsayable in Quantum Mechanics* (Cambridge: Cambridge University Press), pp. 173–180.
- Bell, J. S. (1990), ‘Against “measurement”’, in Miller (1990), pp. 17–31.
- Beller, M. (1999), *Quantum Dialogue: The Making of a Revolution* (Chicago: University of Chicago Press).
- Belousek, D. W. (1996), ‘Einstein’s 1927 unpublished hidden-variable theory: its background, context and significance’, *Studies in History and Philosophy of Modern Physics* **27**, 437–461.
- Bohm, D. (1951), *Quantum Theory* (Englewood Cliffs: Prentice-Hall).
- Bohr, N. (1949), ‘Discussion with Einstein on epistemological problems in atomic physics’, in P. A. Schilpp (ed.), *Albert Einstein: Philosopher-Scientist*, The Library of Living Philosophers, vol. VII (La Salle: Open Court), pp. 201–241.
- Born, M. (1926a), ‘Zur Quantenmechanik der Stossvorgänge’, *Zeitschrift für Physik* **37**, 863–867.
- Born, M. (1926b), ‘Quantenmechanik der Stossvorgänge’, *Zeitschrift für Physik* **38**, 803–827.
- Born, M. (1926c), ‘Das Adiabatenprinzip in der Quantenmechanik’, *Zeitschrift für Physik* **40**, 167–192.
- Born, M., and Wiener, N. (1926), ‘Eine neue Formulierung der Quantengesetze für periodische und nichtperiodische Vorgänge’, *Zeitschrift für Physik* **36**, 174–187.
- Darrigol, O. (1992), *From c-numbers to q-numbers: The Classical Analogy in the History of Quantum Theory* (Berkeley: University of California Press).
- Dirac, P. A. M. (1926), ‘On the theory of quantum mechanics’, *Proceedings of the Royal Society A* **112**, 661–677.
- Dirac, P. A. M. (1927), ‘The physical interpretation of quantum dynamics’, *Proceedings of the Royal Society A* **113**, 621–641.
- Einstein, A., Podolsky, B., and Rosen, N. (1935), ‘Can quantum-mechanical description of physical reality be considered complete?’, *Physical Review* **47**, 777–780.
- Frenkel, V. Y. (1996), *Yakov Ilich Frenkel: His Work, Life and Letters* (Boston: Birkhäuser).
- Heisenberg, W. (1926), ‘Schwankungserscheinungen und Quantenmechanik’, *Zeitschrift für Physik* **40**, 501–506.

- Heisenberg, W. (1927), 'Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik', *Zeitschrift für Physik* **43**, 172–198.
- Heisenberg, W. (1930), *The Physical Principles of the Quantum Theory*, translated by C. Eckart and F. C. Hoyt (Chicago: University of Chicago Press; reprinted New York: Dover, 1949).
- Heisenberg, W. (1948), 'Der Begriff der "Abgeschlossenen Theorie" in der modernen Naturwissenschaft', *Dialectica* **2**, 331–336.
- Heisenberg, W. (1985), 'Ist eine deterministische Ergänzung der Quantenmechanik möglich?', in W. Pauli, *Wissenschaftlicher Briefwechsel mit Bohr, Einstein, Heisenberg u.a., Band II: 1930–1939*, ed. K. v. Meyenn, with the cooperation of A. Hermann and V. F. Weisskopf (Berlin and Heidelberg: Springer), pp. 409–418.
- Holland, P. R. (2005), 'What's wrong with Einstein's 1927 hidden-variable interpretation of quantum mechanics?', *Foundations of Physics* **35**, 177–196.
- Howard, D. (1990), "'Nicht sein kann was nicht sein darf", or the prehistory of EPR, 1909–1935: Einstein's early worries about the quantum mechanics of composite systems', in Miller (1990), pp. 61–111.
- Jordan, P. (1927a), 'Über quantenmechanische Darstellung von Quantensprüngen', *Zeitschrift für Physik* **40**, 661–666.
- Jordan, P. (1927b), 'Über eine neue Begründung der Quantenmechanik, I', *Zeitschrift für Physik* **40**, 809–838.
- Jordan, P. (1927c), 'Über eine neue Begründung der Quantenmechanik, II', *Zeitschrift für Physik* **44**, 1–25.
- Mehra, J., and Rechenberg, H. (2000), *The Historical Development of Quantum Theory*, vol. 6, part 1 (New York: Springer).
- Miller, A. I. (ed.) (1990), *Sixty-two Years of Uncertainty* (New York: Plenum Press).
- Pais, A. (1982), *Subtle is the Lord: The Science and the Life of Albert Einstein* (Oxford: Oxford University Press).
- Pauli, W. (1979), *Wissenschaftlicher Briefwechsel mit Bohr, Einstein, Heisenberg u.a., Teil I: 1919–1929*, eds. A. Hermann, K. v. Meyenn and V. F. Weisskopf (Berlin and Heidelberg: Springer).
- Peres, A. (1993), *Quantum Theory: Concepts and Methods* (Dordrecht: Kluwer).

# 15 Early Impact of Quantum Physics on Chemistry: George Hevesy's Work on Rare Earth Elements and Michael Polanyi's Absorption Theory

GABOR PALLO

According to the standard history, the influence of quantum physics upon chemistry started in 1927. This was the publication year of Heitler and London's seminal article on the hydrogen molecule, an article that is supposed to have radically changed the theory of chemistry and endangered its independence.<sup>1</sup> Since then, many people have considered chemistry as a kind of applied physics, more precisely, of quantum physics. Meanwhile, to researchers working in less theoretical fields of chemistry, such as synthetic organic chemistry or classical chemical analysis, might have remained unnoticed that their discipline disappeared as it had been reduced to physics. In their eyes, chemistry seemed entirely different from physics, even if quantum physics exerted important impact upon its theoretical parts. In the followings, I will detail two cases of the early 1920s to show this impact. The underlying intention of this paper is to demonstrate the non-reductive heuristic value of quantum physics inside chemistry. I emphasize that 'inside chemistry' because the central characters of the two stories are not physicists but chemists, George von Hevesy and Michael Polanyi.<sup>2</sup>

The statement that Hevesy and Polanyi were not physicist but chemists, tacitly includes (to use Polanyi's phrase) that a sharp boundary existed between physics and chemistry, hence we can decide whether someone stands in one or the other side of the boundary. In a scrutiny, however, the boundary problem seems related to reductionism, to the questioned independent status of chemistry. After some general historical remarks on this issue, I will recapitulate the discovery of a chemical element, hafnium, and the interpretation of gas adsorption. The hafnium story is related to the old quantum theory while the absorption theory to quantum mechanics. In both cases, we will see fervent scientific controversies.

---

<sup>1</sup>W. Heitler, F. London, "Wechselwirkung neutraler Atome und homöopolare Bindung nach der Quantenmechanik. *Zeitschrift für Physik*. 44. 1927. 455–472.

<sup>2</sup>Some recent biographies of Hevesy and Polanyi: Siegfried Niese, *Georg von Hevesy: Wissenschaftler ohne Grenzen*. Dresden: Forschungszentrum Rossendorf, 2005. William T. Scott, Martin X. Moleski, S.J., *Michael Polanyi: Scientist and Philosopher*, Oxford: Oxford University Press, 2005.

## Theoretical Chemistry or Applied Physics

Chemistry, and probably other disciplines too, has always had to carry on boundary works, to use Thomas Gieryn's term, meaning that it had to take efforts to demarcate its territory both from physics and biology.<sup>3</sup> Looking back as far as to the 31st Query of Newton's *Optics*, or to the chemical revolution, chemistry's relation with physics has been uneasy.<sup>4</sup> The boundary problem between physics and chemistry can be connected with physicalism, a positivist philosophical stand. In the 19th century, chemical concepts had been attempted to interpret in the framework of mechanics, thermodynamics or electricity. Concepts, such as affinity, valence, chemical bond, later spectroscopy, reaction kinetics, electrochemistry appeared to be very close to physical notions. In an ideal situation, the chemical concepts were assumed to be derivable from the first principles of theoretical physics. On the other hand, many fields of chemistry, including synthetic organic chemistry, were nearer to a particular laboratory practice than to an Aristotelian ideal of science relying on first principles.

Sociologically, the boundaries of chemistry were set by special jobs, by professional university departments providing degrees of chemistry, by textbooks, journals, scientific societies, highly admired researchers, professors, such as Lavoisier, Dalton or Berzelius and their scientific schools, by particular results and tenets like the periodic system created in 1869.<sup>5</sup> By all these means, the discipline of chemistry defined a territory with boundaries worth defending and occasionally extending.

Quantum physics attacked the boundaries both of biology and chemistry. In his work titled *What is life*, Erwin Schrödinger initiated a research program aiming at explaining biological phenomena in a reductionist way, similarly to the way quantum physics explains microphysical phenomena.<sup>6</sup> Max Delbrück and others became supporters of this program that brought major breakthroughs in biology.<sup>7</sup>

Quantum physics entered chemistry with Stark and Einstein's second law of photochemistry in 1912. The first fundamental results were achieved in 1913 by Niels Bohr's model of the atom, and his explanation of the periodic table, to which he returned in 1921–23.<sup>8</sup> Although Bohr's theory was considered to be physics, chemists liked to use it

<sup>3</sup>Thomas Gieryn, *Cultural Boundaries: of Science: Credibility on the Line*. Chicago, London: Chicago University Press, 1999.

<sup>4</sup>A vast amount of literature discussed this problem. See, e.g., Evan M. Melhado, "Chemistry, Physics, and the Chemical Revolution," *Isis* 76. 1985. 195–211.

<sup>5</sup>Mary Jo Nye analyzed the general features of disciplines, mainly chemistry, through their identities. Mary Jo Nye, *From Chemical Philosophy to Theoretical Chemistry: Dynamics of Matter and Dynamics of Disciplines, 1800–1950*. Berkeley, Los Angeles, London: University of California Press, 1993.

<sup>6</sup>E. Schrödinger, *What is Life?* Cambridge: Cambridge University Press, 1944.

<sup>7</sup>In the vast literature see, e.g., D. Fleming, "Émigré Physicists and the Biological Revolution." In: D. Fleming, B. Bailyn, *The Intellectual Migration: Europe and America, 1930–1960*. Cambridge (Mass.): Harvard University Press, 152–189.

<sup>8</sup>N. Bohr, *On the Constitution of Atoms and Molecules* (Papers reprinted from the *Philosophical Magazine* with an introduction by L. Rosenfeld). Copenhagen and New York: Munksgaard and W. A. Benjamin. On the later results see N. Bohr, "The Structure of the Atom," (Nobel Lecture, December 11, 1922.) *Nobel Lectures, Physics, 1922–1941*. Amsterdam: Elsevier Publishing Company, 1965. About the extension of Bohr's building-up theory to molecules, see Buhm Soon Park, "A Principle written in Diagrams: The Aufbau Principle for Molecules and its Visual Representations. 1927–1932." In: U. Klein (ed.), *Tools and Modes of Representation in the Laboratory Sciences*, Dordrecht, Boston, London: Kluwer Academic Publishers, 2001. 179–98.

for interpreting chemical phenomena, because of the model's simplicity and because to a large extent it relied on chemical experimental data.

The radical reductionist program evolved after the introduction of quantum mechanics. In 1929, soon after the publication of Heitler and London's seminal article, Paul Dirac pronounced a radical reductionist program, saying that "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."<sup>9</sup>

Indeed, based on Heitler and London's initial ideas, Slater and Pauling with others established the so-called valence-bond theory, VB in 1927. Hund and Mulliken published the rival theory, called molecular orbital, MO, theory in the same year. In the VB method, hydrogen molecule was considered as an aggregate of two distinct hydrogen atoms, in which the two electrons constituting the chemical bond were placed between the two nuclei. The atoms were distinct physical systems and the theory described their connection. The MO theory, on the other hand, considered the hydrogen molecule as one physical system, having two electrons in one orbital around the two nuclei. The two approaches have competed in quantum chemistry for decades.<sup>10</sup>

Historians Ana Simoes and Kostas Gavroglu, however, pointed at another distinction. In the 1930s, Linus Pauling, a follower of Heitler and London's VB method, used the notion of resonance for explaining traditional organic chemistry problems, such as the tetravalency of carbon, the aromatic structure of benzene, the three-electron bond, and the like. By these, Pauling became part of the structural chemistry tradition rather than the tradition of theoretical physics. Simoes attributed this position partly to Pauling's ties with a research program initiated by Gilbert N. Lewis. Lewis suggested that the atoms composing a molecule could share electron pairs that secure the covalent bond between them. The other factor was a kind of pragmatism, manifested in the so-called 'semi empirical' method. This procedure combined theoretical, quantum physical calculations with empirical data of chemistry, instead of sticking to the physical goals of deriving chemistry from first principles. Simoes and Gavroglu argued that Pauling and Mulliken started a non-reductionist, chemistry-oriented version of quantum chemistry that was rooted in the American pragmatism.<sup>11</sup>

No wonder: Lewis, Pauling and Mulliken were trained as chemists. If quantum chemistry was a fence at the boundary between physics and chemistry, Heitler and London, and most of their followers were sitting on the fence with legs toward physics, while Mulliken and Pauling with legs toward chemistry.<sup>12</sup>

---

<sup>9</sup>P.A.M. Dirac, "Quantum Mechanics of Many Electron Systems," *Proceedings of the Royal Society of London*, A123 (1929): 714–733, on 714

<sup>10</sup>On the history of quantum chemistry see Mary Jo Nye, ref. 5. p. 227–261.

<sup>11</sup>A. Simões, "Chemical Physics and Quantum Chemistry in the Twentieth Century." In Mary Jo Nye (ed), *The Modern Physical and Mathematical Sciences. The Cambridge History of Science*, Vol. 5. Cambridge: Cambridge University Press, 2003. 394–412., A. Simões, K. Gavroglu, "Issues in the History of Theoretical and Quantum Chemistry, 1927–1960." In: C. Reinhardt (ed.), *Chemical Sciences in the 20th Century*. Weinheim: Wiley-VCH, 2001., and K. Gavroglu, A. Simões, "The Americans, the Germans, and the beginnings of quantum chemistry: The confluence of diverging traditions." *Historical Studies in the Physical Sciences*, 25(1), 1994, 47–110.

<sup>12</sup>Buhm Soon Park emphasized that quantum chemistry gradually put on a technical, computational character with a diminishing physical relevance. Buhm Soon Park, "Computational Imperatives in Quantum Chemistry," Paper presented at the HQ-1 conference, July 2–6, 2007, Berlin.



## The Discovery of Hafnium

Encyclopaedia Britannica presented the standard history of the hafnium's discovery as follows: "Bohr pointed out that the missing element 72 would be expected, from its position in the periodic system, to be similar to zirconium in its properties rather than to the rare earths; this observation led G. de Hevesy and D. Coster in 1922 to examine zirconium ores and to discover the unknown element, which they named hafnium."<sup>13</sup>

In this account, Bohr's theory concerning the periodic table was corroborated by Hevesy and Coster. This presentation of the story follows the logic of a reductionist and Popperian philosophy. Indeed, Popper wrote: "all attempts to find it [the chemical element with atomic number 72] were in vain until Bohr succeeded in predicting several of its properties by deducing them from his theory."<sup>14</sup> At another place, Popper said that "it [the discovery of hafnium] struck us then as the great moment when chemistry had been reduced to atomic theory."<sup>15</sup>

From Bohr's point of view, the problem was that while working on the electronic building-up of the atoms in the periodic system, he had to place the still unknown element 72 somewhere in the periodic system. He faced with the dilemma whether the this element was a rare earth to be placed in a separate row below the table with the other rare earths or it was a transition metal to be placed on the table. From his theory, Bohr concluded that element 72 was a transition metal because of its electronic structure.

In his method, by proceeding forward in the periodic table to successive atoms an extra electron should be added to the previous ones. The electrons were arranged in shells and outer shell received the next coming electron. Arriving at the element 57 (see Table 15.1), lanthanum, however, the electrons did not continue to fill the outer *P* shell. Instead, the added electron was placed on the inner *O* shell, *5d*, and in the following elements, starting with cerium, the *N* shell, *4f*, were built up, while the *O* and *P* shells remained unchanged. Fourteen electrons fulfilled the *4f* shell. Hence, the last element belonging to this group should be 71, lutetium, because  $57$  (element number of lanthanum)  $+ 14 = 71$ . The configuration of the outer shell determines the chemical properties of the elements. Since the outer shell of the elements  $57 - 71$  did not change, only inner shells changed, the chemical properties of these elements should be almost identical. These are the rare earth elements. After the *4f* shell has been fulfilled at element 71, the next electron goes to the *O* shell, *5d*, again, making the properties of the unknown element 72 different from the previous ones. Therefore, element 72, should not be a rare earth, and it should be placed on the main table with the transition metals.

From chemical point of view, the historical process seemed different, because the logic of chemical research on rare earths was influenced by the changing methods of analytical chemistry, rather than physical ideas. As historian of analytical chemistry, Ferenc Szabadváry pointed out, rare earths were found mainly in two minerals, yttria and ceria. The chemical properties of rare earths proved almost identical with each other. Moreover, they occurred together in these two minerals. Hence, to separate them (that started in 1787) was extremely difficult and uncertain. This is why their discovery fol-

---

<sup>13</sup>[HTTP://WWW.BRITANNICA.COM/NOBELPRIZE/ARTICLE-80831](http://www.britannica.com/nobelprize/article-80831)

<sup>14</sup>K. Popper, *The Logic of Scientific Discovery*. London: Hutchinson, 1959. p. 69.

<sup>15</sup>K. Popper, *The Open Universe*. London: Hutchinson, 1982. Cited by Eric Scerri, "Popper's Naturalized Approach to the Reduction of Chemistry," *International Studies in the Philosophy of Science*, 12. 1998. 33-44. p. 34.

## Early Impact of Quantum Physics on Chemistry: Hevesy and Polanyi

Number	Element	<i>K</i>	<i>L</i>	<i>M</i>	<i>N</i>	<i>O</i>	<i>P</i>
56	Barium	2	8	18	18	8	2
57	Lanthanum	2	8	18	18	9	2
58	Cerium	2	8	18	19	9	2
59	Praseodymium	2	8	18	21	8	2
60	Neodymium	2	8	18	22	8	2
61	Promethium	2	8	18	23	8	2
62	Samarium	2	8	18	24	8	2
63	Europium	2	8	18	25	8	2
64	Gadolinium	2	8	18	25	9	2
65	Terbium	2	8	18	27	8	2
66	Dysprosium	2	8	18	28	8	2
67	Holmium	2	8	18	29	8	2
68	Erbium	2	8	18	30	8	2
69	Thulium	2	8	18	31	8	2
70	Ytterbium	2	8	18	32	8	2
71	Lutetium	2	8	18	32	9	2
72	Hafnium	2	8	18	32	10	2
73	Tantalum	2	8	18	32	11	2

Table 15.1: Electron configuration of some atoms.

lowed a pattern of division: some components were held to be new chemical elements, but subsequently they proved to be mixtures, the components of the mixture were thought to be elements, but one of them proved to be a mixture, and so on. For instance, in 1905, Auer von Welsbach, an Austrian chemist, applied fractional crystallization of the double oxalates and found out that an element called ytterbium was in fact a mixture of two elements. The French professor Georges Urbain used his own method, based on a ‘separating element’ that crystallizes with rare earth elements, and came to the same conclusion. They simultaneously discovered element 71, lutetium. Chemists found new and new rare earth elements and their final number was uncertain. In 1911, Urbain announced to find a new element mixed with lutetium. He called it celtium, the element 72, another rare earth. In 1922, Urbain with a co-author confirmed the existence of celtium by Roentgen spectroscopy.<sup>16</sup>

This confirmation caused severe headache to Bohr, who wanted to present his new interpretation of the periodic system in his Noble lecture in 1902. He explained the problem to his friend, George de Hevesy, a chemist working in the Bohr institute. Supposing that element 72 was homologue with zirconium, Hevesy with his colleague, the physicist Dirk Coster, analyzed a Norwegian zirconium mineral, by Roentgen spectroscopy and found the unknown element number 72, subsequently named hafnium. Hevesy separated hafnium and proved that it had no rare earth chemical properties.<sup>17</sup>

<sup>16</sup>Ferenc Szabadváry, “The History of the discovery and Separation of the Rare Earth,” In K. A. Gschneider, Jr., L. Eyring, Handbook of the Physics and Chemistry of Rare Earths, Vol. 11. Amsterdam: Elsevier Science Publisher, 1988. 33–80.

<sup>17</sup>Hevesy told this story many times, including his biographical notes that were published with insignificant corrections by J. D. Cockroft as an obituary of Hevesy. J. D. Cockroft: “George de Hevesy

The result of this controversy<sup>18</sup> seems to prove the advantage of the physical theory over chemical experimenting. Karl Popper referred to the hafnium story in this context. More recently, however, philosopher Eric Scerri has challenged the reductionist analysis in a non-reductionist framework. His interpretation of hafnium's discovery relies on two arguments. According to the first one, Bohr's model was not a logical precondition for listing element 72 among transition metals. Some chemists, including the Danish Thomsen in 1895, predicted that element 72 would be homologous with zirconium. After knowing the results of Moseley's Roentgen spectroscopy measurements carried out in 1914, this place appeared doubtless. According to the other argument, which seems stronger in our context, the discovery of hafnium does not support reductionism, because the Bohr model itself was not a deductive result from first principles. Scerri argued that this model, the old quantum theory was inductive relying on various experimental facts, many originating in chemistry.<sup>19</sup>

Indeed, in the tradition of chemistry, the discovery of hafnium is attributed to George Hevesy, a chemist. This exemplary case neither proves, nor falsifies the potential reduction of chemistry to physics but demonstrates an effective collaboration between quantum physics and chemistry.

## Theory of Adsorption

Adsorption is a phenomenon whereby gasses are attracted and stuck to the surface of a solid. Michael Polanyi did pioneering but controversial research on adsorption. His ideas might originate in the biographical contingency that Polanyi graduated from medicine, obtaining limited training in chemistry. He worked out the basic elements of his potential theory of adsorption, while being hospitalized in Budapest, in 1914, without any access to the current scientific literature.<sup>20</sup>

As he did not know about the electronic theory of chemical processes, Polanyi based his interpretation of adsorption on classical thermodynamics. He thought that the van der Waals type attractive forces originated in the surface of solids establish a potential gradient. Polanyi called this force adsorption potential, and assumed that it influenced the gas above the adsorbent in a way that was similar to compression. By the work done by adsorption potential, the gas was thought to condense in an adsorbed phase upon the surface of the solid. Adsorption potential was defined by a simple formula:  $\varepsilon = f(\varphi)$ , in which  $\varepsilon$  is the adsorption potential,  $\varphi$  is the space where the force is effective. In this model, the adsorbed layers of gas were several molecules thick.<sup>21</sup>

---

1885–1966", Biographical Memoirs of Fellows of the Royal Society, 13. 1967, 125–166. D. Coster, G. Hevesy, "On the new element hafnium." *Nature*, 111. 1923. 182, and 252. After working out the details of the hafnium chemistry, Hevesy published a monograph on the new element: G. Hevesy, *Das Element Hafnium*. Berlin: Springer, 1927.

<sup>18</sup>About the controversy, see H. Kragh, "Anatomy of a priority conflict: The case of element 72." *Centaurus*. 23. 1980. 275–301.

<sup>19</sup>E. Scerri, "Prediction of the Nature of Hafnium from Chemistry, Bohr's Theory and Quantum Theory." *Annals of Science*. 51. 1994. 137–150.

<sup>20</sup>About Polanyi's life, see W. T. Scott, M. X. Moleski, S.J. , *Michael Polanyi: Scientist and Philosopher*. Oxford: Oxford University Press, 2005.

<sup>21</sup>M. Polanyi, "Adsorption, Quellung und osmotischen Druck von Kolloiden," *Biochemische Zeitschrift*, 66. 1914. 258–268., M. Polányi, "Über Adsorption und Kapillarität vom Standpunkte des II. Hauptsatzes," *Zeitschrift für physikalische Chemie*, 88. 1914. 622–631., M. Polanyi, "Über die Adsorption

This consequence of Polanyi's potential theory of adsorption met serious disagreements. In 1921, living already in Germany, Polanyi was invited to give an account of his theory at the seminar of the Kaiser-Wilhelm Institute for Physical Chemistry and Electrochemistry.<sup>22</sup> Characteristically, the chemist audience, including Herbert Freundlich, head of department and expert of adsorption, or Hermann Mark, found Polanyi's theory convincing because it was in harmony with the experimental data available then.<sup>23</sup> However, Haber, Nernst and particularly the special guest, Albert Einstein strictly refused it. "I survived the occasion only by the skin of my teeth."—Polanyi remembered in 1963.<sup>24</sup>

The attack was directed against the multimolecular layers of the adsorbed molecules on the adsorbent. The critics thought it was impossible for two reasons. Firstly, because Polanyi had no convincing theory on the nature of the attractive force originated in the surface of the adsorbent. His thermodynamic argumentation was considered old fashioned, which disregarded contemporary results of physics related to the electronic character of the atomic and molecular forces, in particular, disregarded the nature of the dipole interactions. The critics supposed that the van der Waals type forces decreased by an inverse sixth power and that the dipole-dipole forces between the adsorbed molecules were shielded out by the adsorbed molecules. They did not see any force to keep several layers of the adsorbed molecules on the surface of the adsorbent.<sup>25</sup>

Secondly, the criticism referred to Polanyi's negligence of Irving Langmuir's adsorption theory that was launched in 1916 and gradually became main stream. Langmuir relied on the latest physical theories, including electronic structure of matter, electron pairs and chemical bond. In his adsorption theory, Langmuir supposed that electrostatic forces originate in the adsorbent, which are related to the valence of the molecules on the surface of the adsorbent. Because of the range of this force, the gas molecules can only constitute a monomolecular layer on the surface of the adsorbent. Langmuir published an isotherm equation, the widely used Langmuir isotherm, and supported his theory by elegant experimental results. Polanyi's rival proved so persuasive that he received the 1932 Chemistry Nobel Prize.<sup>26</sup>

In spite of Einstein and Haber's criticism and Langmuir's success, Polanyi was convinced about the value of his theory, even if was based on a 19th century physical picture. His supposedly victorious argument came from quantum theory. Fritz London,

---

vom Standpunkt des dritten Wärmesatzes," Verhandlungen der deutschen physikalischen Gesellschaft, 16. 1914. M. Polányi: Adsorption von Gasen (Dampfen) durch ein festes nichtflüssiges Adsorbens. Verhandlungen der deutschen physikalischen Gesellschaft, 18. 1916. 55–80. 1012–1016. Polanyi's PhD Theses: Polányi Mihály, Gázok (gozök) adsorbtiója szilárd, nem illanó adsorbensen. Doktori disszertáció. 30 o. Budapest, 1917.

<sup>22</sup>About Polanyi's times in Berlin see Mary Jo Nye, "Historical Source of Science-as-a-social-practice: Michael Polanyi in Berlin," *Historical Studies in the Physical and Biological Sciences*, 37. 2. 2007. 409–434.

<sup>23</sup>The chemists' favorable reaction was reported in an interview with Hermann Mark. W. T. Scott, M. X. Moleski, S.J. , Michael Polanyi, ref. 19. p. 74.

<sup>24</sup>M. Polanyi, "The Potential Theory of Adsorption", *Science*, 141. 1963. 1010–3. Reprinted in: M. Polanyi, *Knowing and Being*. London: Routledge & Kegan Paul, 1969. p. 97–104.

<sup>25</sup>W. T. Scott, M. X. Moleski, S.J. , Michael Polanyi, ref. 19. p. 73.

<sup>26</sup>Langmuir's fundamental paper: I. Langmuir, "The adsorption of gases on plane surfaces of glass, mica and platinum", *Journal of the American Chemical Society*, 40. 1918, 1361–1403. A wider view: I. Langmuir, "Surface chemistry", Nobel Lecture, December 14, 1932. [HTTP://NOBELPRIZE.ORG/NOBEL-PRIZES/CHEMISTRY/LAUREATES/1932/LANGMUIR-LECTURE.HTML](http://nobelprize.org/nobel_prizes/chemistry/laureates/1932/langmuir-lecture.html)

one of the physicist founders of quantum chemistry, after moving to Berlin at the end of the 1920s, regularly participated in the seminars at Haber's institute. By then Polanyi was a leading researcher of the institute, the head of a section, out of two sections of the institute. (The other section's head was Herbert Freundlich, chemist, an expert of adsorption.) In 1930, London published a quantum mechanical calculation on a weak force, called dispersion force, working between two dipoles.<sup>27</sup> From Polanyi's point of view dispersion force had two particularly important features. Firstly, it was not electric, therefore, shielding out does not occur. Secondly, its range above the adsorbent decreased by an inverse third power, rather than sixth powers as in the case of the van der Waals type forces, meaning that the range of dispersion force was much larger than the range of the van der Waals force. It seemed large enough to create more than one layers on the surface of the adsorbent. Polanyi cooperated with London in calculating the dispersion force working in the case of adsorption and they could identify dispersion force with Polanyi's adsorption potential, just the way he described in his study it in 1914 and 1916.<sup>28</sup> With his collaborators in Haber's institute, mainly H. Goldman, Polanyi created an apparatus for experimental research of adsorption by which they thought they confirmed the potential theory and the multilayer image of adsorption.

According to William Scott, Polanyi's biographer, in the early 1930s Polanyi felt great satisfaction seeing his original theory of adsorption to be justified.<sup>29</sup> Historian Mary Jo Nye added that in 1932, Polanyi's colleague, Herbert Freundlich published a paper intending to compromise between the two rival theories. Polanyi thought that Langmuir's formula was a simplistic idealization that can be derived as a special case from his theory. Although he thought that his theory was firm and well founded, Polanyi knew that it did not gain wide acceptance.<sup>30</sup> Scott cited a letter written by Polanyi to a friend: "Whose fate is better, mine or Langmuir's? My theory is absolutely right but not accepted. Langmuir's theory is wrong but very famous... Langmuir is better off." <sup>31</sup>

Polanyi fled to Britain from Hitler in 1933, and gradually changed from chemistry to philosophy. In 1958, he published *Personal knowledge*, a very influential book on the philosophy of science inspired by cultural, moral, political and of course scientific commitments.<sup>32</sup> Indeed, commitment was one of Polanyi's central categories besides tacit knowledge, focal and subsidiary awareness and others. All these served as conceptual instruments to analyze discoveries, rather than justification, unlike the main stream contemporary philosophy of science that divided scientific research between the context of justification and discovery. Discovery was considered contingent, psychological, and sociological, an inappropriate subject for rational philosophical reflections. Polanyi thought

---

<sup>27</sup>F. London, "Theorie und Systematik der Molekularkräfte," *Zeitschrift für Physik*, 63. 1930. 245–279., F. London, "Properties and applications of molecular forces", *Zeitschrift für Physikalische Chemie (B)*, 11. 1930. 222–251. R. Eisenschitz, F. London, "Über das Verhältnis der van der Waalsschenkräfte zu den homoopolaren Bindungskräften," *Zeitschrift für Physik*, 60. 1930. 491.

<sup>28</sup>F. London, M. Polanyi, "Über die atomtheoretische Deutung der Adsorptionskräfte," *Die Naturwissenschaften*, 18. 1930. 1099–1100.

<sup>29</sup>W. T. Scott, M. X. Moleski, S.J. , Michael Polanyi, ref. 19. p. 126.

<sup>30</sup>Mary Jo Nye, "Michael Polanyi's Theory of Surface Adsorption: How Premature?," In: E. B. Hooke (ed.), *Prematurity in Scientific Discovery: On Resistance and Neglect*. Berkeley: University of California Press, 2002. 151–164.

<sup>31</sup>W. T. Scott, M. X. Moleski, S.J. , Michael Polanyi, ref. 19. p. 112.

<sup>32</sup>M. Polanyi, *Personal Knowledge*. London: Routledge and Kegan Paul, 1958; Chicago: Chicago University Press 1958.

that scientific ideas were born before research, as a kind of preliminary knowledge or belief, and research in fact articulates, justifies the ideas instead of producing them. Therefore, the precondition of a good research work is to believe in an idea that emerges in the course of doing science. His whole philosophy was about and based on belief and commitment whether speaking about science, epistemology, ethics, religion, or esthetics.

Although Polanyi worked out his philosophy several decades later than he had received criticism from his peers concerning his potential theory of adsorption, one cannot resist thinking that his behavior was motivated by his deep belief in and commitment to the multilayer model. When working it out, he was a young researcher, just left his country behind, lacking any shelter, any family or colleagues network, working on a field, physical chemistry, without proper basic training and receiving sharp criticism from leading experts of science. Polanyi needed that strong belief and commitment to his belief for not giving up, not fleeing from science. He was looking for justification. In 1963, remembering his adventure with the potential theory of adsorption, Polanyi wrote in *Science* that after the criticism he had received “my belief in my theory was quite unshaken...”.<sup>33</sup> He continued in this way: “I became immune to these objections, but I remained powerless to refute them.”<sup>34</sup> Eugen Wigner, Polanyi’s student had a different impression. He thought even Polanyi might have some doubts concerning his own theory of adsorption: “The writer of these lines [Wigner] remembers that when he pointed to some experimental data strongly supporting the multilayer character of adsorption, Polanyi was quite taken aback.”<sup>35</sup>

According to Mary Jo Nye, by 1930 after about twenty years research work “the old-fashioned potential gradient now had a firm theoretical basis in the new quantum mechanics.”<sup>36</sup> By that time, however, the Langmuir approach rooted deeply in physical chemistry. Nevertheless, potential theory of adsorption stayed alive. Both Mary Jo Nye and William Scott showed that the theory found its way in the textbooks of chemistry. I can add that in the 1950s and 60s, the Hungarian physical chemistry and colloid chemistry textbooks also contained detailed descriptions of it with modernized versions, including that of M. Dubinin.<sup>37</sup> Multilayer adsorption theory has finally been accepted in the main stream.

## Conclusions

The two cases, the histories of the discovery of hafnium and the potential theory of adsorption did not exemplify the reduction of chemistry to physics, although in both cases quantum physics played a crucial role. In both cases, chemistry seemed helpless in deciding controversial issues. A renowned authority in the field of rare earth chemistry,

---

<sup>33</sup>M. Polanyi, “The Potential Theory of Adsorption”, ref 23. p. 89.

<sup>34</sup>Ibid. p. 91.

<sup>35</sup>E. P. Wigner, R. A. Hodgkin, “Michael Polanyi, 12 March 1891 – 22 February, 1976,” *Biographical Memoirs of Fellows of the Royal Society*, 23. 1977. 412–448.

<sup>36</sup>T. Erdey-Gruz, G. Schay, *Elméleti Fizikai Kémia (Theoretical Physical Chemistry)*, Budapest: Tankönyvkiado, 1952–1954. The potential theories of adsorption are discussed (in the fourth edition published in 1964) in Vol. 2. p. 389–400. E. Wolfram, *Kolloidika*, (lecture notes for chemistry students of the Eötvös Lorand University) Budapest: Tankönyvkiado, 1965. p. 156–159.

<sup>37</sup>Mary Jo Nye, “At the Boundaries: Michael Polanyi’s Work on Surfaces and the Solid State,” In: C. Reinhardt (ed.), *Chemical Sciences in the 20th Century*. Weinheim: Wiley-VCH, 2001. p. 249.

George Urbain concluded that element 72 was a rare earth, while some other chemists thought it was not. None of the arguments were entirely convincing to the chemical community that inclined to accept Urbain's position concerning cerium. Bohr's quantum theory was not considered decisive for chemists. However, Bohr's theory provided strong arguments to Hevesy to search for hafnium in a non rare earth mineral. In chemistry, the preparation of the new element counted as the strongest argument for the existence of this element, and the derivation from the first principles of physics did not matter very much. Bohr's model was not an attack against the border of chemistry, rather a useful heuristic instrument that helped chemists to interpret chemical phenomena, even after the model proved fallacious.

The history of adsorption showed some similar features. In working out his potential theory, Polanyi relied on the classical thermodynamics used by physical chemistry that he learned in Budapest mainly from Walter Nernst's book, *Theoretical Chemistry*.<sup>38</sup> Polanyi's approach was criticized referring to a pre-quantum mechanical view of molecular forces. Polanyi's adsorption potential gained solid theoretical foundation from quantum physics, sixteen years after its construction. However, in this case, foundation did not mean a deduction from first principles. The disadvantage of Polanyi's theory was that it failed to produce an equation for adsorption isotherms. Such a formula would have been considered a real analytical approach in the sense of physicalism. Adsorption has not been deduced from quantum physics or quantum chemistry, but it could be interpreted by it. Consequently, potential theory of adsorption remained behind the boundaries of physical chemistry, while it needed the quantum theoretical interpretation.

Our two cases revealed that quantum physics could play important role in chemistry without completely reducing it to physics. Sociologically, this was expressed by the cooperative efforts in our cases. Simoes and Gavroglu described the differences between the early German and American quantum chemistry schools in terms of the main character's relationship with chemistry, finding that the German quantum chemistry community consisted of physicists, while the Americans of chemists.<sup>39</sup> Our cases showed that in the European continent, including Germany fruitful cooperation was established between the two fields. In the case of hafnium, the chemist Hevesy cooperated with the physicist Bohr, in adsorption theory the chemist Polanyi with the physicist Fritz London. The representatives of the two disciplines walked to the boundary from two different directions and proceeded together peacefully along the border without any sorrow fight.

---

<sup>38</sup>W. T. Scott, M. X. Moleski, S.J. , Michael Polanyi, ref. 19. p. 25. Probably, it was an edition of Walther Nernst, *Theoretische Chemie vom Standpunkte der Avogadro'schen Regel und der Thermodynamik*. Stuttgart: Verlag von Ferdinand Enke, 1st edition, 1893.

<sup>39</sup>K. Gavroglu, A. Simões, "The Americans, the Germans, and the beginnings of quantum chemistry: The confluence of diverging traditions," *Historical Studies in the Physical Sciences*, 25(1). 1994. 47–110.

# 16 Computational Imperatives in Quantum Chemistry

BUHM SOON PARK

In the traditional narrative of the history of quantum physics, the problem of chemical binding appears only briefly at the end of the long march toward the formulation of a new mechanical system. This is usually introduced as one of the exemplary problems that quantum mechanics solved, thereby validating its general applicability. Singularly recognized as ground-breaking is Walter Heitler and Fritz London's 1927 paper, which gave a theoretical explanation of why two hydrogen atoms combine to form a molecule.<sup>1</sup> Thereafter, Heitler and London were optimistic about understanding the whole territory of chemistry with quantum mechanics, and their reductionist ideal was shared by other physicists, including P. A. M. Dirac, who made a famous statement that "the underlying physical laws for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known."<sup>2</sup> Indeed, the excitement about the new theoretical framework was abundant in the late 1920s, as the historian Max Jammer put it: "Satisfied that the theory "works," since it provided unambiguous answers whenever invoked, physicists engaged themselves rather in solving problems which so far had defied all previous attempts or which promised to open up new avenues of research." According to him, Heitler and London's work "eventually brought the whole of chemistry under the sovereignty of quantum mechanics."<sup>3</sup>

Intriguing is the fact that historians of quantum physics, including Jammer, have paid little attention to whether the reductionist program worked well or faced difficulties in chemistry after 1927. They tend to believe that quantum chemistry, a new field of study that came into being after Heitler and London's paper, would successfully carry the mission of reducing chemistry to physics. Historians of quantum chemistry are rather critical of this picture. They have shown that the early optimism about reductionism quickly subsided into pessimism in the 1930s in the face of complexity of chemical systems, and that quantum chemistry was developed into a discipline with diverse methodologies, indigenous languages, and separate institutional bases.<sup>4</sup> To them, the acceptance of quantum mechanics in chemistry does not necessarily mean the re-

<sup>1</sup>Walter Heitler and Fritz London, "Wechselwirkung neutraler Atome und homöopolare Bindung nach der Quantenmechanik," *Zeitschrift für Physik*, **46** (1927), 455–72.

<sup>2</sup>P. A. M. Dirac, "Quantum Mechanics of Many-Electron Systems," *Proceedings of the Royal Society*, **A123** (1929), 714–33, quote on p. 714.

<sup>3</sup>Max Jammer, *The Conceptual Development of Quantum Mechanics*, 2nd ed. (College Park, MD: American Institute of Physics, 1989), pp. 359–60, 384–86.

<sup>4</sup>Kostas Gavroglu and Ana I. Simões, "The Americans, the Germans, and the Beginnings of Quantum Chemistry: The Confluence of Diverging Traditions," *Historical Studies in the Physical and Biological Sciences*, **25** (1994), 47–110; Mary Jo Nye, *From Chemical Philosophy to Theoretical Chemistry* (Berkeley: University of California Press, 1993).



duction of one discipline to another. While I agree on this point of view in general, I want to point out that the historians of quantum chemistry have not fully examined, either, the subsequent development of mathematical tools and conceptual devices to solve the Schrödinger equation for multi-electron atomic or molecular systems without using empirical data. This paper aims to reassess the place of the pioneers of *ab initio* methods in the history of quantum physics or quantum chemistry.<sup>5</sup> I first examine who they were, why they got interested in computations, and how they improved agreement between theory and experiment. And then I show that their computation-oriented work was undervalued by some leading scientists, whose attitude has significantly affected the current historiography of quantum physics and chemistry.

### Heitler and London's 1927 Paper

In 1927, two German physicists, Walter H. Heitler and Fritz London, published a paper in which they treated the hydrogen molecule with quantum mechanics and studied the source of its binding energy. This paper was quantum mechanics' first step toward chemistry, almost single-handedly creating the new field of quantum chemistry. In view of the significance of this paper, it is interesting to note that the encounter of Heitler and London was incidental, and that their collaboration was short-lived. Both Heitler and London were products of the University of Munich, trained in different areas: London took his Ph.D. in philosophy in 1921 and spent some years in a teaching job before he decided to study theoretical physics under Sommerfeld; and Heitler worked on the theory of concentrated solutions for his doctoral degree, which he got in 1925, and went to Copenhagen to continue his work on physical chemistry with Niels Bjerrum. Their paths converged in 1927 when each of them received the Rockefeller Fellowship and went to Zurich to learn wave mechanics under Schrödinger. After publishing their joint paper, Heitler and London continued to study the problem of the chemical bond for some years, but subsequently their interests diverged, Heitler moving into the quantum field theory and London into superconductivity.<sup>6</sup>

Heitler and London's basic idea was to regard the molecule as composed of atoms, a view which was not different from the traditional conception of the molecule in chemistry.<sup>7</sup> But Heitler and London adopted it as part of applying the approximation technique known as the perturbation method, which had been developed in celestial mechanics and used in the old quantum theory. Assuming that the atoms were set apart at the infinite internuclear distance, they first approximated the wave function ( $\Psi$ ) of the hydrogen molecule with known eigenfunctions of the hydrogen atom,  $\Psi_1\varphi_2$ , where  $\Psi_1$  was the eigenfunction of electron 1 at nuclei *a* and  $\varphi_2$  was that of electron 2 at nuclei *b*. At this point, the interaction between the atoms could be neglected. However, as the atoms came closer to each other, one could not ignore the interatomic interaction. Heitler and London regarded this interaction among two electrons and two nuclei as the

---

<sup>5</sup>The term *ab initio*, which means "from the beginning," was first used around 1950. Peter W. Atkins, *Quanta: A Handbook of Concepts*, 2nd ed. (Oxford: Oxford University Press, 1991), p. 1.

<sup>6</sup>Nevill F. Mott, "Walter Heinrich Heitler," *Biographical Memoirs of the Fellows of the Royal Society*, **28** (1982), 141–51; and Kostas Gavroglu, *Fritz London: A Scientific Biography* (Cambridge: Cambridge University Press, 1995).

<sup>7</sup>For reactions to Heitler and London's paper, see Gavroglu, *Fritz London*, pp. 51–3; Gavroglu and Simoes, "The Americans, the Germans, and the Beginnings of Quantum Chemistry," pp. 70–75.

perturbation of the system.

Here, Heitler and London found that the perturbation included not only the usual Coulombic interaction between electrons but also a possibility of electron exchange (“Austausch”). For one could not know which electron was located near which nuclei: that is, the electrons were indistinguishable. Therefore,  $\varphi_1\Psi_2$  being as acceptable an approximation of  $\Psi$  as  $\Psi_1\varphi_2$ , the correct representation would be linear combinations of  $\Psi_1\varphi_2$  and  $\varphi_1\Psi_2$ :

$$\Psi_\alpha = \frac{1}{\sqrt{2+2S}}(\Psi_1\varphi_2 + \Psi_2\varphi_1)$$

$$\Psi_\beta = \frac{1}{\sqrt{2-2S}}(\Psi_1\varphi_2 - \Psi_2\varphi_1)$$

where  $S$  (overlap integral) was  $\int \Psi_1\varphi_1\Psi_2\varphi_2 d\tau$ . Putting these values into the Schrödinger equation, where  $R$  is the internuclear distance,  $r_{12}$  the distance between the two electrons,  $r_{a1}$  the distance between the nucleus  $a$  and the electron 1, and so on,

$$\nabla_1^2\Psi + \nabla_2^2\Psi + \frac{8\pi^2m}{h^2} \left\{ E - \left( \frac{e^2}{R} + \frac{e^2}{r_{12}} - \frac{e^2}{r_{a1}} - \frac{e^2}{r_{a2}} - \frac{e^2}{r_{b1}} - \frac{e^2}{r_{b2}} \right) \right\} \Psi = 0,$$

they obtained two different energy levels,  $E_\alpha$  and  $E_\beta$ :

$$E_\alpha = E_{11} - \frac{E_{11}S - E_{12}}{1+S} = \frac{E_{11} + E_{12}}{1+S}$$

$$E_\beta = E_{11} + \frac{E_{11}S - E_{12}}{1-S} = \frac{E_{11} - E_{12}}{1-S}$$

where  $E_{11}$  and  $E_{12}$  were integrals of the following form,

$$E_{11} = \int \left[ \left( \frac{e^2}{r_{12}} + \frac{e^2}{R} \right) \frac{\Psi_1^2\varphi_2^2 + \Psi_2^2\varphi_1^2}{2} - \left( \frac{e^2}{r_{a1}} + \frac{e^2}{r_{b2}} \right) \frac{\Psi_2^2\varphi_1^2}{2} - \left( \frac{e^2}{r_{a2}} + \frac{e^2}{r_{b1}} \right) \frac{\Psi_1^2\varphi_2^2}{2} \right] d\tau$$

$$E_{12} = \int \left( \frac{2e^2}{r_{12}} + \frac{2e^2}{R} - \frac{e^2}{r_{a1}} - \frac{e^2}{r_{a2}} - \frac{e^2}{r_{b1}} - \frac{e^2}{r_{b2}} \right) \frac{\Psi_1\varphi_2\Psi_2\varphi_1}{2} d\tau$$

After obtaining this mathematical expression for the energy of  $H_2$ , Heitler and London considered the physical meaning of  $E_\alpha$  and  $E_\beta$  and their components,  $E_{11}$  and  $E_{12}$ . It was certain that  $E_{11}$  had to do with the “Coulombic interaction of the present charge distribution,”<sup>8</sup> and that this integral could be solved analytically as a function of the internuclear distance,  $R$ . In contrast,  $E_{12}$  did not permit such a simple, classical interpretation as  $E_{11}$  did. Moreover, it was difficult to calculate all the integrals involved in  $E_{12}$ , particularly the one known as the exchange integral,  $\int \frac{\Psi_1\varphi_2\Psi_2\varphi_1}{r_{12}} d\tau$ . Heitler and London circumvented this difficulty by considering only its upper limit, and drew approximate graphs of  $E_\alpha$  and  $E_\beta$ . (see Fig. 18.1)

According to this energy diagram,  $E_\beta$  represented a repulsion between the atoms at any internuclear distance;  $E_\alpha$  showed an attraction at a larger distance and a repulsion at a smaller distance, having a minimum value when the internuclear distance  $R$  was 1.5

<sup>8</sup>Heitler and London, “Wechselwirkung,” 461.

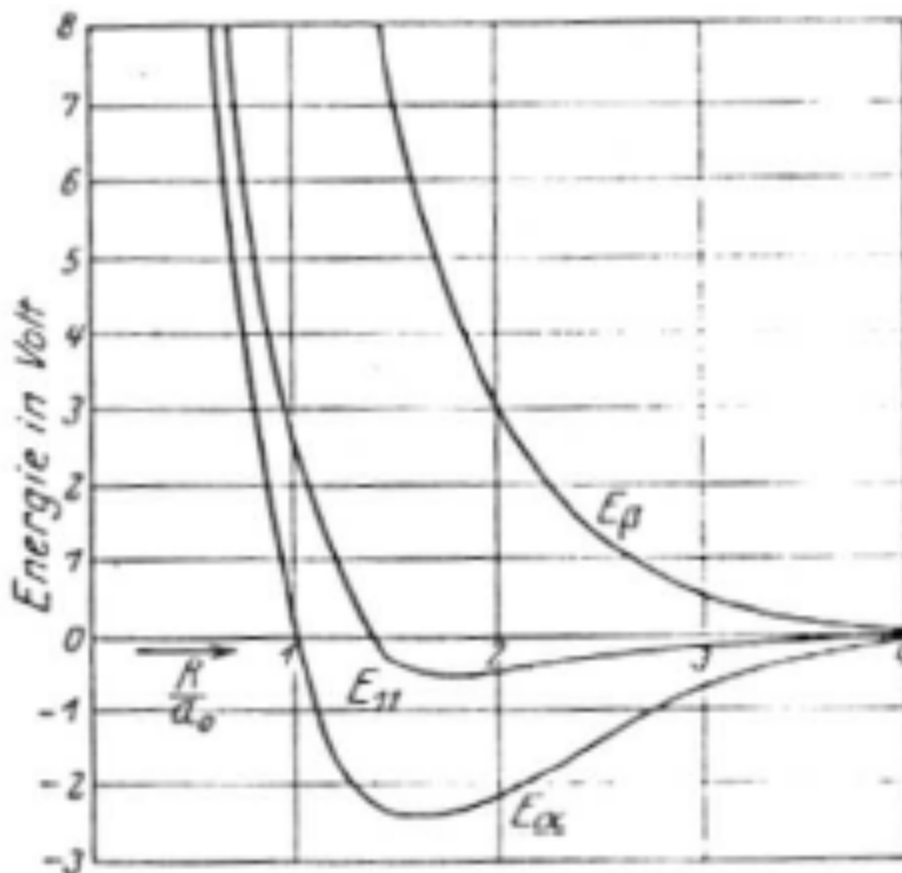


Figure 16.1: Heitler and London's energy diagram of the hydrogen molecule.  $E_\alpha$  represents nonpolar attraction;  $E_\beta$  elastic reflection; and  $E_{11}$  coulomb interaction.

$a_0$  or  $0.8 \text{ \AA}$ . From the graph of  $E_\alpha$ , the corresponding dissociation energy or the binding energy was about  $2.4 \text{ eV}$ .<sup>9</sup>

Heitler and London did not compare their theoretical values with observed ones, presumably because the agreement was not particularly good for the binding energy. But they seemed to place less emphasis on the quantitative argument than on the interpretative promise of their treatment, which explained the attraction between the two *non-polar* hydrogen atoms without considering perturbation by polarization. This was due to the electron exchange, a “characteristic quantum-mechanical effect.” Represented by the integral  $E_{12}$ , the exchange effect affected  $E_\beta$  as the van der Waals repulsion (“elastic reflection”) of two hydrogen atoms; and it contributed to  $E_\alpha$  as the strength of the molecular binding (i.e., the chemical bond).<sup>10</sup>

<sup>9</sup>Kostas Gavroglu and Ana Simões have mistakenly said that Heitler and London obtained  $72.3 \text{ kcal}$  (about  $3.2 \text{ eV}$ ) for the binding energy of the hydrogen molecule. Gavroglu and Simões, “Quantum Chemistry,” p. 63; and Gavroglu, *Fritz London*, p. 47. As I will show, this value was in fact obtained by Yoshikatsu Sugiura, who computed the exchange integral which Heitler and London had roughly estimated.

<sup>10</sup>Heitler and London, “Wechselwirkung,” pp. 460–63.

What was the nature of this exchange effect? Why did non-polar hydrogen atoms interact in two different ways, attraction and repulsion? Heitler and London could conveniently define the frequency of exchange by the energy difference of  $E_\alpha$  and  $E_\beta$  divided by the Planck constant,  $\frac{E_\beta - E_\alpha}{h}$ . But they found it difficult to characterize this effect in the language of classical mechanics. At least, they saw the exchange effect as “closely related with the quantum mechanical resonance phenomenon” introduced by Werner Heisenberg a year earlier for the problem of helium,<sup>11</sup> in that both resonance and exchange originated from the indistinguishability of electrons. Yet Heitler and London noted some subtle differences: “While, in resonance, electrons of different energy levels in the same set of eigenfunctions exchange their energy, here, electrons of the same state (the same energy) yet different eigenfunction systems ( $\Psi$  and  $\varphi$ ) exchange their places.”<sup>12</sup>

The interpretation of  $E_\alpha$  and  $E_\beta$  was important in another way. The Pauli exclusion principle required  $E_\alpha$  to be an energy state in which the electrons were in opposite spin orientations (antiparallel); and  $E_\beta$ , in the same orientation (parallel). Therefore, the electronic spin state was a useful indicator of the molecular formation: the antiparallel spin state led to the attraction (thus, bonding), while the parallel one corresponded to the unstable excited state. In other words, the chemical bond resulted from the pairing of electrons of different spin orientations, and valence was predicated on this pairing. This established a connection between the spin theory of valence and the Lewis theory of paired-electron bond which London elaborated in his papers of 1928.<sup>13</sup>

### Toward Better Agreement between Theory and Experiment

The further development of Heitler and London’s treatment of the hydrogen molecule went in two directions. On the one hand, two Americans, John C. Slater and Linus Pauling, applied Heitler and London’s interpretative scheme to polyatomic molecules, explaining the directed property of valence with the concept of hybridization.<sup>14</sup> On the other hand, there were those who attempted to make the Heitler and London approach acceptable quantitatively as well as qualitatively. They calculated the exchange integral, employed physical and chemical insights to narrow the gap between theory and experiment, and even developed different kinds of computational schemes.

The first step in this direction was made by Yoshikatsu Sugiura, who came from

<sup>11</sup>Werner Heisenberg, “Mehrkörperproblem und Resonanz in der Quantenmechanik,” *Zeitschrift für Physik*, **38** (1926), 411–26. On the origins of the resonance concept in physics and its use in chemistry, see Cathryn Carson, “The Peculiar Notion of Exchange Forces—I: Origins in Quantum Mechanics, 1926–1928,” *Studies in History and Philosophy of Modern Physics* **27** (1996), 23–45; Buhm Soon Park, “Chemical Translators: Pauling, Wheland and Their Strategies for Teaching the Theory of Resonance,” *British Journal for the History of Science*, **32** (1999), 21–46. On Heisenberg’s study of helium, see Jagdish Mehra and Helmut Rechenberg, *The Historical Development of Quantum Theory*, vol. 3: *The Formulation of Matrix Mechanics and Its Modifications, 1925–1926* (New York: Springer-Verlag, 1982), pp. 282–301.

<sup>12</sup>Heitler and London, “Wechselwirkung,” p. 461. For Heitler and London’s concern about (mis)interpretation of exchange effect, see Gavroglu and Simoes, “Quantum Chemistry,” pp. 61–5.

<sup>13</sup>Heitler and London, “Wechselwirkung,” pp. 465–8. Fritz London, “Zur Quantentheorie der homöopolaren Valenzzahlen,” *Zeitschrift für Physik*, **46** (1928), 455–77; and idem, “Zur Quantenmechanik der homöopolaren Valenzchemie,” *Zeitschrift für Physik*, **50** (1928), 25–51.

<sup>14</sup>Buhm Soon Park, “The Contexts of Simultaneous Discovery: Slater, Pauling, and the Origins of Hybridisation,” *Studies in the History and Philosophy of Modern Physics*, **31** (2000), 451–474.

Japan to Europe to learn the new quantum theory in the late 1920s. Thanks to Max Born at Göttingen, Sugiura had an opportunity to read Heitler and London's paper before its publication. Finding that they did not calculate the exchange integral, Sugiura plunged into this problem. In August 1927, he obtained the solution of the integral  $E_{12}$  as a function of the distance between the two atoms through a complex procedure of mathematical manipulation involving a power series expansion.<sup>15</sup>

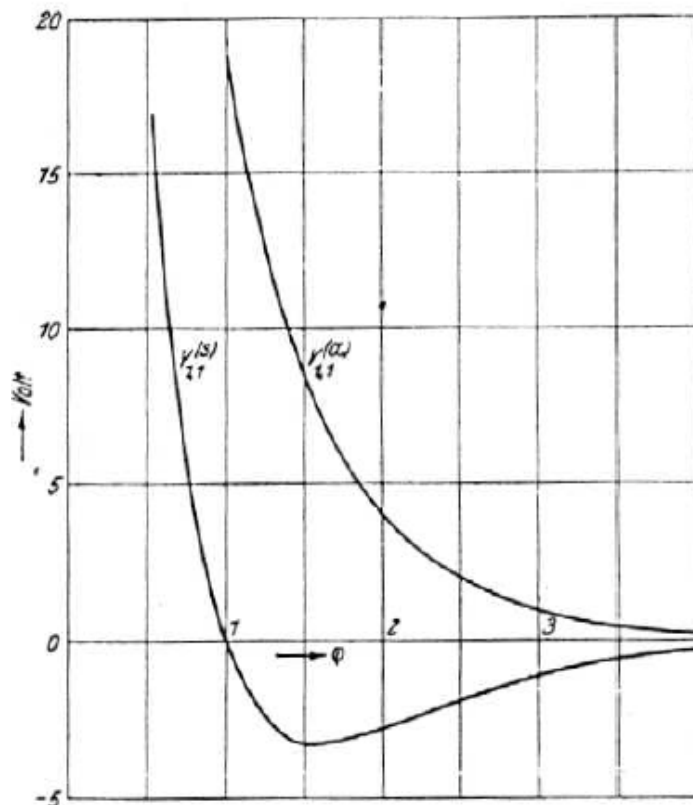


Figure 16.2: Sugiura's energy diagram for the hydrogen molecule: Sugiura's notations of  $V_{1,1}^{(s)}$  and  $V_{1,1}^{(a)}$  correspond to Heitler and London's  $E_{11}$  and  $E_{12}$ .

Sugiura showed that the equilibrium separation of H<sub>2</sub> was the same as Heitler and London's value, 0.8Å. But his calculation of the binding energy was 3.2 eV, which was closer to the then available empirical value, 4.4 eV, than Heitler and London's had been. The agreement was, in his opinion, satisfactory.

Shou Chin Wang, a Chinese physicist studying at the University of Columbia for his doctoral degree, was one of those interested in the problem of the hydrogen molecule. Although his thesis adviser was an old-fashioned mathematical physicist, Wang had a chance to learn quantum mechanics by reading the latest issues of *Zeitschrift für Physik* in a study group led by Ralph Kronig.<sup>16</sup> Wang's approach was basically the same as

<sup>15</sup>Yoshikatsu Sugiura, "Über die Eigenschaften des Wasserstoffmoleküls im Grundzustande," *Zeitschrift für Physik*, **45** (1927), 484–92. On Born's guidance, see *ibid.*, p. 492.

<sup>16</sup>Katherine R. Sopka, *Quantum Physics in America, 1920–1935* (New York: Arno Press, 1980), pp.

Heitler and London's in that he formed a linear combination of wave functions assuming atomic individuality in the molecule.<sup>17</sup> However, Wang attacked the problem with a different mathematical technique. Instead of calculating the perturbation energy, he adopted what had been known as the Ritz method or the variation method, in which one could determine the coefficients of the linear combination in a way that gave the lowest possible energy value. This method had been successfully applied to the problem of helium by the German physicist Georg W. Kellner.<sup>18</sup> In addition, Wang was also attracted to Kellner's use of the effective nuclear charge  $Ze$  as a variable parameter, which took into account the screening effect of electrons over nuclei—the effect that the electronic orbits are contracted into a smaller region because of the Coulombic attraction between electrons and nuclei. Putting the effective nuclear charge into the hydrogen eigenfunctions, Wang finally obtained improved results: the equilibrium separation was 0.73 Å and the dissociation energy 3.76 eV. When he had almost completed his paper, Wang received the latest issue of *Zeitschrift für Physik* containing Sugiura's paper. Nevertheless, Wang was confident that his work was worthy of publication for the reason that he “used a new method of calculation and arrived at some results in a little better agreement with the experimental data than Sugiura's.”<sup>19</sup>

Sugiura and Wang did not attempt to make further improvements of their calculations.<sup>20</sup> But the persistent discrepancy between theory and experiment continued to attract attention from young scientists like Nathan Rosen. Rosen was to be best known later as one of the co-authors of the Einstein-Podolsky-Rosen (EPR) paradox, which was devised to criticize the Copenhagen interpretation of quantum mechanics in 1935. But in the early 1930s, Rosen worked on the problem of  $H_2$  as a graduate student of Slater at MIT. According to Rosen, previous treatments of this problem were “hitherto successful qualitatively but not quantitatively.”<sup>21</sup> He maintained that there should be a better way to inquire as to the various complicated interactions between atoms, such as the distortion of the charge distribution. Rosen valued Wang's treatment of this distortion

---

3.48–3.50, and p. 3.102.

<sup>17</sup>Shou C. Wang, “The Problem of the Normal Hydrogen Molecule in the New Quantum Mechanics,” *Physical Review*, **31** (1928), 579–86.

<sup>18</sup>Georg W. Kellner, “Die Ionisierungsspannung des Heliums nach der Schrödingerschen Theorie,” *Zeitschrift für Physik*, **44** (1927), 91–112.

<sup>19</sup>Wang, “Hydrogen Molecule,” p. 579.

<sup>20</sup>After his research trip in Europe, Sugiura returned to Tokyo to join the Institute of Physical and Chemical Research (Riken), which had been established in 1917, modeled after Germany's Imperial Institute for Physics (Physikalisch-Technische Reichsanstalt). Along with Bunsaku Arikatsu and Woshio Nishina, Sugiura also lectured on quantum mechanics at Kyoto from 1929 to 1931, spreading the “Copenhagen spirit.” Among his students were the future Nobel laureates, Hideki Yukawa and Shinichiro Tomonaga. See Hideki Yukawa, *Tabibito*, trans. L. M. Brown and R. Yoshida (Singapore: World Scientific, 1982), pp. 176–7. For the context for the establishment of Riken, see Itakura Kiyonobu and Yagi Eri, “The Japanese Research System and the Establishment of the Institute of Physical and Chemical Research,” in *Science and Society in Modern Japan*, ed. Nakayama Shigeru, David L. Swain, and Yagi Eri (Cambridge: MIT Press, 1974), pp. 158–201. In comparison, Wang continued to study the new quantum mechanics and atomic theory at Wisconsin and Chicago on a National Research Fellowship in 1928–29. Like Sugiura, however, he finally went back to his own country, China, to teach modern physics at the University of Chekiang and later at Peking University. For Wang's professional career, see National Research Council, *National Research Fellowships, 1929–1944* (Washington, D.C.: National Research Council, 1944), p. 37.

<sup>21</sup>Nathan Rosen, “The Normal State of the Hydrogen Molecule,” *Physical Review*, **38** (1931), 2099–114, quote on 2099.

with the altered atomic radius; but to him, it was “rather far from the goal.” Noting that atomic interactions might occur along the molecular axis rather than symmetrically about a sphere, he assumed that the electronic cloud of an atom would be polarized or “bulge out” toward its binding partner. His consideration of the “polarization effect” gave an improved value of the binding energy, 4.02 eV.

By the early 1930s, it had been known that one of the weaknesses in the Heitler and London approach was its neglect of the possibility of ionic configurations in molecules. Sidney Weinbaum examined this problem under the guidance of Pauling at the California Institute of Technology (Caltech). He added ionic terms to wave functions originally proposed by Heitler and London, finding an improvement in the binding energy of 0.0031 eV or 3 percent over Sugiura’s value.<sup>22</sup> He also showed that the consideration of the effective nuclear charge plus the ionic term would yield an improvement of 8 percent over Wang’s value, a result which was almost equivalent to Rosen’s. The addition of Rosen’s term into the Wang-ionic treatment turned out to give the best value, 4.10 eV, among the ones obtained by Heitler and London’s method.

In 1933, Hubert M. James and Albert S. Coolidge obtained by far the most accurate theoretical value, using the coordinate of the interelectronic distance, the method developed by the Norwegian physicist Egil Hylleraas for helium.<sup>23</sup> James and Coolidge were at Harvard University: James as a physics graduate student working toward his doctoral degree, and Coolidge as a chemistry professor. Though from different departments, they had a common background in that both learned quantum mechanics in Edwin C. Kemble’s lectures. And their initial collaboration took place, at Kemble’s suggestion, when they checked each other’s calculations for quantum mechanical treatments of the chlorine molecule (by James) and the water molecule (by Coolidge).<sup>24</sup> During his calculations, James found that  $Cl_2$  was too complex to be handled by the Heitler and London method, and thus changed his problem to a much simpler one, that of the lithium molecule. Here, he soon realized that “all calculations made up to that time on molecules with inner shells [like  $Li_2$ ] were unreliable, some apparently good results being due to cancellation of several serious approximations.” This time, James looked for a better method of approximation. “I completed this work [on  $Li_2$ ] in the summer of 1932. while I was on vacation at my home in West Virginia,” he recalled. “The result brought me to look for a better method than that of Heitler and London for the treatment of molecules, and I naturally did this in the context of the simplest typical molecule,  $H_2$ .”<sup>25</sup>

James and Coolidge abandoned the fundamental assumption of the Heitler and London method, i.e., the atomic individuality. Instead of approximating the molecular wave function with the atomic eigenfunctions, they started with a trial function having many

---

<sup>22</sup>Sydney Weinbaum, “The Normal State of the Hydrogen Molecule,” *Journal of Chemical Physics*, **1** (1933), 593–6.

<sup>23</sup>Hubert M. James and Albert S. Coolidge, “The Ground State of the Hydrogen Molecule,” *Journal of Chemical Physics*, **1** (1933), 825–35.

<sup>24</sup>In fact, Hubert M. James started his graduate study in the chemistry department in 1928. But after finding that his interests were in mathematics and physics, he switched over to the physics department. For James’s switch and Kemble’s role in the James-Coolidge collaboration, see James to Spencer R. Weart, May 1980, American Institute of Physics Early 1930s Ph.D. Project, “Hubert James,” MB 31484.

<sup>25</sup>James to Sopka, 9 May 1972, quoted in Sopka, *Quantum Physics*, pp. 4.87–4.88.

variable parameters:

$$\Psi = \sum_{mnjkp} C_{mnjkp} \left[ \frac{1}{2\pi} e^{-\delta(\lambda_1 + \lambda_2)} \left( \lambda_1^m \lambda_2^n \mu_1^j \mu_2^k \rho^p + \lambda_1^n \lambda_2^m \mu_1^k \mu_2^j \rho^p \right) \right]$$

where  $\lambda_1$ ,  $\lambda_2$ ,  $\lambda_3$ , and  $\lambda_4$  were four elliptic coordinates of the following relations,

$$\lambda_1 = \frac{r_{1a} + r_{1b}}{R}$$

$$\lambda_2 = \frac{r_{2a} + r_{2b}}{R}$$

$$\mu_1 = \frac{r_{1a} - r_{1b}}{R}$$

$$\mu_2 = \frac{r_{2a} - r_{2b}}{R}$$

and the fifth coordinate,  $\rho = \frac{2r_{12}}{R}$ , had the interelectronic distance in it. The summation was to extend over the positive or zero values of the indices, with the restriction that  $j+k$  must be even, which was required by nuclear symmetry. The function was also able to take as many terms as necessary to give an acceptable approximation for the energy. To examine the behavior of this function, James and Coolidge fixed the equilibrium distance ( $R$ ) at  $1.4 a_0$  (or  $0.74 \text{ \AA}$ ), and the exponent ( $\delta$ ) at  $0.75 a_0$ , and then solved a set of equations which came from the condition of making values of the  $C$ 's minimize the energy.

It turned out that the inclusion of several terms could lead to an energy value much better than any previously reported. As the number of terms increased, the improvement slowed. The computations became more and more laborious, because the incorporation of each new term required the computation of numerous integral terms. The success of James and Coolidge's treatment was immediately recognized as a "thoroughly satisfactory treatment of the normal hydrogen molecule, the only improvement which we may look forward to being the increase in accuracy by the inclusion of further terms."<sup>26</sup> And their paper was also praised as showing that Schrödinger's equation was reliable for molecules as well as atoms. Charles A. Coulson later said, "It is not unreasonable to claim that their highly laborious calculations, yielding such an excellent final result, represent one of the most satisfactory 'proofs' of the validity of the original wave equation when applied to problems with more than one electron."<sup>27</sup>

James and Coolidge's success was a source of optimism that molecular properties could be computed with only the Schrödinger equation and several fundamental constants, such as the electronic charge ( $e$ ), the electronic mass ( $m_e$ ), Planck's constant ( $h$ ), the atomic number ( $Z$ ), and the masses of the nuclei involved, with no further empirical data. In another sense, however, James and Coolidge's success was a source of pessimism: the amount of computation was simply formidable. Thus textbook writers of quantum chemistry noted:

<sup>26</sup>Pauling and Wilson, *Quantum Mechanics*, p. 351.

<sup>27</sup>Charles A. Coulson, *Valence* (Oxford: Clarendon Press, 1952), p. 118. See also Henry F. Schaefer III, *Quantum Chemistry: The Development of Ab Initio Methods in Molecular Electronic Structure Theory* (Oxford: Clarendon Press, 1984), pp. 1-2.



Type of Wave Function	Maximum Binding Energy ( $D_e$ )	Equilibrium Separation ( $r_e$ )
Heitler-London, rough estimation (Heitler and London, 1927)	2.4	0.8
Heitler-London, computed (Sugiura, 1927)	3.14	0.87
Heitler-London with screening (Wang, 1928)	3.76	0.73
Heitler-London with screening + polarization term (Rosen, 1931)	4.02	0.74
Heitler-London + ionic term (Weinbaum, 1933)	3.21	0.90
Heitler-London with screening + ionic term (Weinbaum, 1933)	4.00	0.74
Heitler-London with screening + polarization term + ionic term (Weinbaum, 1933)	4.10	-
Trial Function with the interelectronic coordinate (James and Coolidge, 1933)		
one term	2.56	0.74
five terms	4.507	0.74
eleven terms	4.682	0.74
thirteen terms	4.697	0.74
Experiment	4.725	0.74

Table 16.1: Quantum-mechanical calculations of the binding energy and equilibrium separation of the hydrogen molecule from 1927 to 1933. Source: John H. Van Vleck and Albert Sherman, “The Quantum Theory of Valence,” *Reviews of Modern Physics*, **7** (1935), 167–228. The molecular orbital approximation performed poorly even with the consideration of the screening effect. See Charles A. Coulson, *Valence* (Oxford: Clarendon Press, 1952), p. 119.

However, the labor involved in these calculations is so great even for these simple systems [like He,  $H_2^+$ , and  $H_2$ ] that it does not appear to be a profitable method of attack on molecular problems in general. Because of the mathematical difficulties involved, we are forced to use much less accurate approximations; usually we are forced to write the wave function as some linear combination of one-electron wave functions. Although these will not give satisfactory quantitative results, they should in general be qualitatively correct, and should enable us to correlate experimental chemical facts.<sup>28</sup>

As James found, “a good fortune” of unjustified approximations could provide remarkably good results for diatomic molecules, such as  $Li_2$ ,  $LiH$ ,  $Na_2$ ,  $K_2$ , and  $KH$ .<sup>29</sup> One of the often used assumptions was to consider only the valence electrons, that is, to ignore the other electrons in the closed inner shells, when dealing with the binding energy of molecules larger than hydrogen. Neglect of the inner-shell electrons gave a nice

<sup>28</sup>Henry Eyring, John Walter, and George E. Kimball, *Quantum Chemistry* (New York: John Wiley & Sons, 1944), p. 217.

<sup>29</sup>Hubert M. James, “Wave-Mechanical Treatment of the  $Li_2$  Molecule,” *Journal of Chemical Physics*, **2** (1934), 794–810; and idem, “Wave-Mechanical Treatment of the Molecule  $Li_2^+$ ,” *Journal of Chemical Physics*, **3** (1935), 9–14. See also John H. Van Vleck and Albert Sherman, “The Quantum Theory of Valence,” *Reviews of Modern Physics*, **7** (1935), 167–228, esp. 185–6.

agreement between the calculated and observed values of the binding energy of  $Li_2$ , but James showed that the consideration of inner-shell electrons would completely destroy the agreement. The rigorous treatment gave poorer results than the rough one! It was called “the nightmare of inner shells.”<sup>30</sup> In fact, James proposed a remedy for this problem: describe valence electrons with the same function as he and Coolidge had devised for hydrogen, and treat non-valence electrons by means of simple atomic orbitals. However, computational difficulties in this procedure, especially considering  $r_{12}$  terms in the presence of other electrons, were insurmountable. James could only conclude: “In principle, then, we appear to have a way in which to treat diatomic molecules with any desired precision. Unfortunately, the limits of human patience restrict the usefulness of the complete method.”<sup>31</sup>

James and Coolidge continued their collaboration until 1940, working on polyatomic molecules, but with no notable success.<sup>32</sup> Their research program demanded intensive labor with the then available computing facilities. It was only after the war that human patience was greatly relieved by the development of electronic digital computers<sup>33</sup>; and the field of rigorous computations of molecular properties was then opened up again. But James and Coolidge, like other workers involved in the H<sub>2</sub> problem, never returned to the field. Paradoxically, James and Coolidge’s work heralded the coming of the “dark ages” of the *ab initio* method.<sup>34</sup>

### From Helium to Many-Electron Atoms

The point of departure for the problem of many-electron atoms was, as always, the normal helium atom: various approximation methods were first developed and tested for helium before being applied to larger atoms. The criteria for testing a method, in view of its further applicability, included the amount of labor in computations as well as the degree of accuracy of computed results. The desideratum was that approximations would make problems “manageable” without the expense of accuracy; but that was difficult to achieve.

By 1930, an outstanding agreement between theory and experiment on the helium

---

<sup>30</sup>Van Vleck and Sherman, “Quantum Theory of Valence,” pp. 185–6.

<sup>31</sup>Ibid., pp. 186–90, quote on p. 190. This part of the review article was written by James. See footnote 37.

<sup>32</sup>James to Weart, May 1980, American Institute of Physics Early 1930s Ph.D. Project, “Hubert James,” MB 31484. In 1940, James became an assistant professor at Purdue University, where his interests were diverted to polymer and solid-state physics.

<sup>33</sup>Buhm Soon Park, “The ‘Hyperbola of Quantum Chemistry’: The Changing Identity and Practice of a Scientific Discipline in the Early Years of Electronic Digital Computers, 1945–65,” *Annals of Science* **60** (2003), pp. 219–247.

<sup>34</sup>Schaffer, *Ab Initio Methods*, p. 4. Indeed the quantitative investigation of molecules, being limited to relatively simple ones, languished in the late 1930s and 40s. Only a small number (seven) of studies on the hydrogen molecule were reported in this period, and all of them, using various trial functions, fell short of the accuracy of James and Coolidge’s. See A. D. McLean, A. Weiss, and M. Yoshimine, “Configuration Interaction in the Hydrogen Molecule-The Ground State,” *Reviews of Modern Physics*, **32** (1960), 211–8. Andrea I. Woody also points out the difficulty of applying James and Coolidge’s method to other molecules, and sketches the development of the Configuration Interaction method after the war. Andrea I. Woody, “Early Twentieth Century Theories of Chemical Bonding: Explanation, Representation, and Theory Development (Quantum Chemistry)” (Ph.D. Diss., University of Pittsburgh, 1997).

problem had been achieved by Egil A. Hylleraas.<sup>35</sup> Hylleraas took his Ph.D. at the University of Oslo in 1924, working on the crystal lattice theory. Two years later, after spending the intervening period as a school teacher, he joined Born's group at Göttingen on a Fellowship of the International Education Board in the hope of furthering his work on crystals. But, following Born's suggestion, Hylleraas decided to study problems related to the application of quantum mechanics.<sup>36</sup> At that time, the basic understanding of the spectral properties of helium had been well established by Heisenberg; but there was still a broad gap between the spectroscopic measurement of the ionization energy (24.46 eV) and its numerical calculation, either by the old quantum theory (28 eV) or by a simple perturbation treatment of the Schrödinger equation, as given by Albrecht Unsöld (20 eV).<sup>37</sup> The introduction of an effective nuclear charge by Geroge Kellner reduced the discrepancy from about 4 to 1.5 eV,<sup>38</sup> which was still a significant amount. Under Born's guidance, Hylleraas began to attack the problem of helium with a noisy electric desk calculator called the Mercedes Euclid to handle a large volume of numerical work. Using a trial function that might be interpreted as representing one electron in an inner orbit and the other in an outer orbit, Hylleraas obtained a good result, 24.35 eV. It was soon "greatly admired and thought of as almost a proof of the validity of wave mechanics, also, in the strict numerical sense."<sup>39</sup> Not fully satisfied with this result, however, Hylleraas continued to work on reducing the discrepancy after his return to Oslo. Finally, he made a major advance by introducing in the wave function a new coordinate of the interelectronic distance,  $u = \frac{r_{12}}{a_0}$ , which occurred in the interaction term for the two electrons. The final theoretical value for the energy of the helium atom was only 0.0016 eV below the experimental value: a discrepancy like this could be attributed to a numerical error in the calculations or to experimental error or possibly to some small effects such as electron-spin interactions, motion of the nucleus, and so on.<sup>40</sup> It was seen as a triumph for quantum mechanics when applied to many-electron atoms, as Linus Pauling and E. Bright Wilson put it: the "success of this program would strengthen our confidence in our wave-mechanical equations, and permit us to proceed to the discussion of many-electron atoms and molecules."<sup>41</sup>

And yet it was not easy to adapt Hylleraas's method to heavy atoms, because the number of terms that had to be computed increased very rapidly with increasing numbers of electrons. Even in the early 1960s, no successful application of the method was reported for atoms heavier than lithium, a three-electron system.<sup>42</sup> However, the intro-

<sup>35</sup>Egil A. Hylleraas, "Über den Grundzustand des Heliumatoms," *Zeitschrift für Physik* **48** (1928): 469–94; idem, "Neue Berechnung der Energie des Heliums in Grundzustande, sowie des tiefsten Terms von Orthohelium," *Zeitschrift für Physik*, **54** (1929), 347–66; and idem, "Über den Grundterm der Zweielektronenprobleme von  $H^-$ , He,  $Li^+$ ,  $Be^{++}$  usw.," *Zeitschrift für Physik*, **65** (1930), 209–225.

<sup>36</sup>For Hylleraas's educational background and Born's influence upon him, see Egil A. Hylleraas, "Reminiscences from Early Quantum Mechanics of Two-Electron Atoms," *Reviews of Modern Physics*, **35** (1963), 421–31.

<sup>37</sup>Albrecht Unsöld, "Beiträge zur Quantenmechanik der Atome," *Annalen der Physik*, **82** (1927), 355–93.

<sup>38</sup>Kellner, "Ionisierungsspannung des Heliums," pp. 91–112.

<sup>39</sup>Hylleraas, "Grundzustand des Heliumatoms," pp. 469–94. The quote is from Hylleraas, "Reminiscences," p. 427.

<sup>40</sup>Linus Pauling and E. Bright Wilson, *Introduction to Quantum Mechanics With Applications to Chemistry* (New York: McGraw-Hill Book Company, 1935), p. 224.

<sup>41</sup>Ibid., pp. 222–4.

<sup>42</sup>John C. Slater, "The Electronic Structure of Atoms—The Hartree-Fock Method and Correlation," *Reviews of Modern Physics*, **35** (1963), 484–7.

duction of  $r_{12}$  was not the only method for considering the inter-electronic interaction known as *electronic correlation*. Hylleraas was also a pioneer of another method called the *configuration interaction*. Instead of approximating the “true” wave function with one-electron functions, he devised a way of using a set of functions of any number, possibly an infinite number.<sup>43</sup> But the computational difficulty with this method, along with the modest result, discouraged him from proceeding further.

Less accurate but more applicable than Hylleraas’s two methods was the use of wave functions of the simple, analytic form which might relieve the labor of computations. The hydrogen eigenfunctions—the solutions of the Schrödinger equation for the hydrogen problem—were such functions; and, in fact, they were exact solutions for other atomic problems when the interaction between the electrons was entirely neglected. Kellner partially took care of this interaction in helium, by putting an effective nuclear charge into the function and fixing its value with the variation principle. This technique was soon applied to lithium and the other elements in the first row of the periodic table,<sup>44</sup> where, instead of the original wave functions of hydrogen, their asymptotic form (a form at large distances between a nucleus and electrons) was used. The modified wave functions had the same angular part as the hydrogen counterparts had, but their radial part,  $r^{n^*-1} e^{-\left[\frac{(Z-s)r}{n^*}\right]}$ , was different in that it had no radial nodes. Here  $r$  was the distance between nucleus and electron,  $n^*$  the effective quantum number (the parameter for the principle quantum number),  $Z$  the nuclear charge, and  $s$  the screening constant. In 1930 Slater used this form of wave function to discuss the size, the ionization potential, and magnetic properties of much heavier atoms like Fe and Co. Hence the name the Slater-Type Orbitals (STOs). Yet Slater did not determine the screening constants and other parameters with the variation principle, but adjusted them using empirical values. His was the semi-empirical study of atomic properties. Slater thus said: “It is to be hoped that eventually a variation calculation can be made here too; but we may anticipate that the figures given in this paper will be substantially verified, and in the meantime, an approximate set of functions is much better than none.”<sup>45</sup>

Another approach was developed by the Englishman Douglas R. Hartree in 1928, called the Self-Consistent-Field (SCF) method. As it turned out, the SCF method was less accurate but much more manageable than Hylleraas’s; and it was more laborious but much more reliable than the method of using analytical functions. Hartree was a Cambridge man, who was born and educated, taught, and died in Cambridge.<sup>46</sup> He excelled in mathematics at St. John’s College, Cambridge, graduating in 1921 with First Class Honors in Part I of the Mathematical Tripos and Second Class Honors in Part

<sup>43</sup>Egil A. Hylleraas, “Über den Grundzustand des Heliumatoms,” *Zeitschrift für Physik*, **48** (1928), 469–94.

<sup>44</sup>Victor Guillemin, Jr. and Clarence Zener, “Über eine einfache Eigenfunktion für den Grundzustand des Li-Atoms und der Ionen mit drei Elektronen,” *Zeitschrift für Physik*, **61** (1930), 199–205; and Clarence Zener, “Analytic Atomic Wave Functions,” *Physical Review*, **36** (1930), 51–6.

<sup>45</sup>John C. Slater, “Atomic Shielding Constants,” *Physical Review*, **36** (1930), 57–64, quote on p. 57.

<sup>46</sup>C. G. Darwin, “Douglas Rayner Hartree,” *Biographical Memoirs of the Fellows of the Royal Society*, **4** (1958), 103–16; and R. B. Lindsay, “Douglas Rayner Hartree,” in *Dictionary of Scientific Biography*, vol. 6, ed. Charles C. Gillispie (New York: Charles Scribner’s Sons, 1970), pp. 147–8. See also Ana Simões and Kostas Gavroglu, “Quantum Chemistry in Great Britain: Developing a Mathematical Framework for Quantum Chemistry,” *Studies in the History and Philosophy of Modern Physics*, **31** (2000), 511–48.

II of the Natural Sciences Tripos. Hartree continued his graduate study in Cambridge under the Plummer Professor of Mathematical Physics, Ralph H. Fowler. A highlight of that time was Bohr's visit to Cambridge in 1921. Immediately attracted to the quantum theory as presented by one of its authors, Hartree began to explore the electronic structure of atoms. It was the problem that Bohr handled only qualitatively. If Bohr's theory was right, Hartree pondered, could one find an electric field for the atom?—the field in which one could draw the actual form of the orbits and course of time along it, and furthermore in which one could calculate the energy levels of states matching experimental data. In 1923 Hartree sought to answer this question in his paper, "On Some Approximate Numerical Applications of Bohr's Theory of Spectra."<sup>47</sup>

As Hartree set out in the introduction, this paper contained a germ of the idea of the "self-consistent-field."

For various reasons a type of field is assumed much simpler than the actual atomic field must be, and exact agreement between all calculated and observed terms is not to be expected and cannot in fact be obtained, but good enough agreement is obtained to make the quantitative results interesting; and both for the dimensions of the orbits and for the field they probably form a fairly good first approximation. The orbits of the electrons normally present in the atom having been calculated, the field due to them could be determined and compared with the field deduced from the spectral terms.<sup>48</sup>

His logic was clear: (1) assume a simple type of field (here, a central field, i.e., a function of the distance  $r$  from the nucleus only); (2) impose quantum conditions on this field; (3) express the effective nuclear charge  $Z$  as a function of  $r$ , and solve the integral for the field,  $V$  ( $V = \int^{\infty} \frac{Z}{r^2} dr$ ); (4) compare the obtained field with the experimental one, to see if they are consistent. In reality, however, Hartree could not obtain the atomic field only from the theory. Instead, he worked backwards, reversing steps (3) and (4): he put empirical energy terms into the equation obtained from the quantum conditions, and then found  $Z$  as an empirical function of  $r$ . Since the  $Z$  function was given only in a graphical or tabular form, the final integration had to be carried out numerically.

Hartree's method here was semi-empirical. But, within the framework of the old quantum theory, there were not many alternatives for getting a quantitative picture of the electric field of atoms.<sup>49</sup> Moreover, his study indicated a notable paradox of the Bohr theory: the electrons moving *in sharply defined orbits* produced a *smooth charge distribution curve*, which went quite a long way outside the boundary of the atom.<sup>50</sup> This was explained only after the arrival of quantum mechanics.

Hartree was awarded his Ph.D. in 1926, but he stayed in Cambridge as a Fellow of St. John's College and of Christ's College until he took the Chair of Applied Mathematics

---

<sup>47</sup>Douglas R. Hartree, "On Some Approximate Numerical Applications of Bohr's Theory of Spectra," *Proceedings of the Cambridge Philosophical Society*, **21** (1923), 625–41.

<sup>48</sup>Ibid., p. 625.

<sup>49</sup>Hartree acknowledged that E. Fues did similar calculations independently, but argued that his own method was more general than Fues' was. See Ibid. In 1924, R. B. Lindsay sought to derive a charge density straightforwardly from a spherical average of Bohr orbits, which Slater saw as a step closer to the self-consistent-field method. See John C. Slater, *Solid-State and Molecular Theory: A Scientific Biography* (New York: John Wiley & Sons, 1975), p. 53.

<sup>50</sup>Hartree, "Numerical Applications," p. 639. See also Slater, "Structure of Atoms," p. 485.

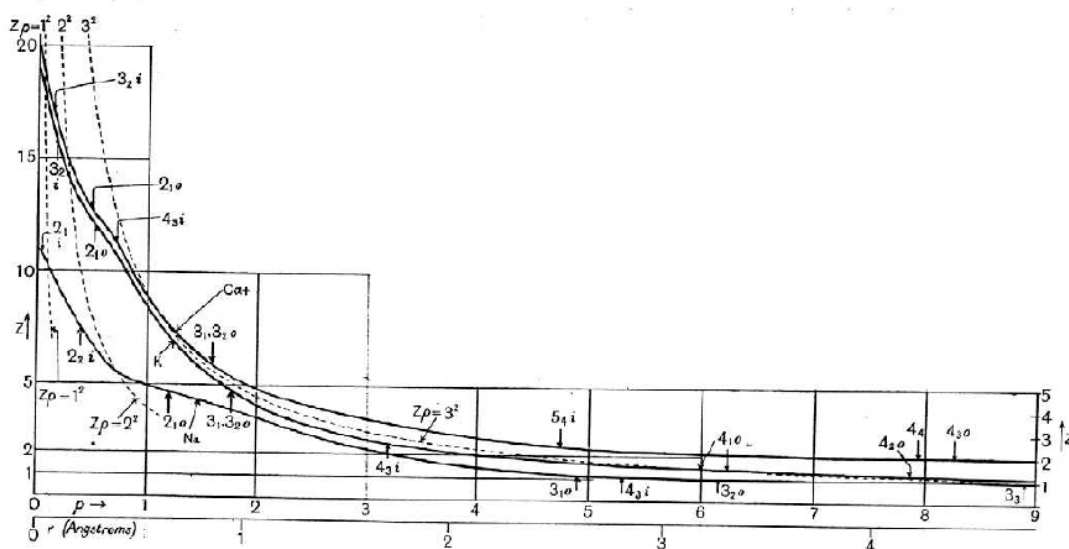


Figure 16.3: Hartree's early idea of the Self-Consistent-Field method.  $(Z, \rho)$  curves for  $Na$ ,  $K$ ,  $Ca^+$ , determined by analysis of optical and X-ray spectral terms.  $Z$  is the effective nuclear charge, and  $\rho$  is the distance from nucleus in Bohr's atomic unit (that is,  $\frac{r}{a}$ , where  $a$  is the radius of hydrogen). The full line curves are the curves of  $Z$  as a function of  $\rho$ . The broken curves are the hyperbolae  $Z\rho = k^2$  ( $k$ , the radial quantum number, is the integer).

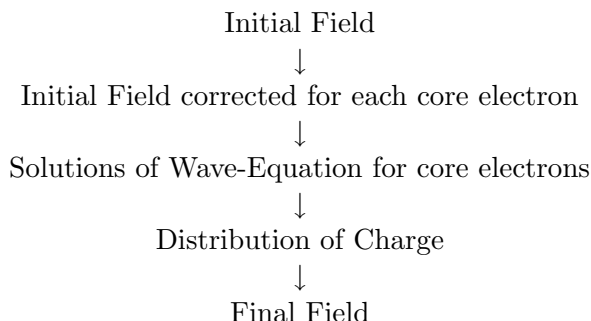
at the University of Manchester in 1929. It was in this postdoctoral period that Hartree developed a quantum-mechanical method of investigating the electronic structure of atoms.<sup>51</sup>

The overall structure of Hartree's new method looked similar to that of his old one.<sup>52</sup> First of all, Hartree started by assuming a central field (of the function of  $r$  only), which he called the "initial field." He then corrected the field for each electron, as the distributed charge of an electron must be omitted in finding the field acting on it. The third step was to put this corrected field into the Schrödinger equation and solve it for each electron. From the solutions for all electrons, a distribution of charge could be calculated. Hartree then found the field of the nucleus and this charge distribution, the "final field."

<sup>51</sup>Douglas R. Hartree, "The Wave Mechanics of an Atom with a Non-Coulomb Central Field. Part I. Theory and Methods," *Proceedings of the Cambridge Philosophical Society*, **24** (1928), 89–110; idem, "The Wave Mechanics of an Atom with a Non-Coulomb Central Field. Part II. Some Results and Discussion," *Proceedings of the Cambridge Philosophical Society*, **24** (1928), 111–32; idem, "The Wave Mechanics of an Atom with a Non-Coulomb Central Field. Part III. Term Values and Intensities in Series in Optical Spectra," *Proceedings of the Cambridge Philosophical Society*, **24** (1928), 426–37; and idem, "The Wave Mechanics of an Atom with a Non-Coulomb Central Field. Part IV. Further Results Relating to the Optical Spectrum," *Proceedings of the Cambridge Philosophical Society*, **25** (1929), 310–15.

<sup>52</sup>"Wave Mechanics. Part II," pp. 111–4.

He summarized the procedure with the following diagram for a core electron:



If the final field was the same as the initial field, the field would be called “self-consistent”; and no more numerical work would be necessary. If not, one should repeat the same procedure by using the final field of the first approximation as the initial field of the second one, over and over again, until self-consistency would be achieved.

Therefore, unlike the old quantum theory, quantum mechanics enabled Hartree to obtain the atomic charge distribution without using any empirical data. He needed no input of spectral information to calculate the energy level of atoms. The SCF method was non-empirical, *ab initio*. This feature was the major difference between the SCF method and his previous one. As an example, Hartree showed how successive approximations narrowed the difference between the effective nuclear charge of initial and final field for rubidium (Rb), an atom having thirty-seven electrons.<sup>53</sup>

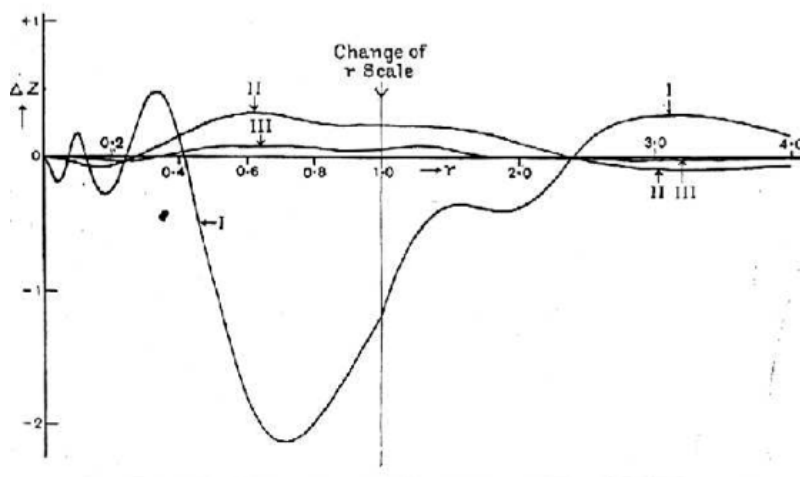


Figure 16.4: Hartree’s three approximations to Self-Consistent-Field for Rb. Difference  $\Delta Z$  between effective nuclear charge of initial and final field was plotted against  $r$  for the three approximations (Curves I, II, and III).

In general, Hartree was satisfied with the agreement between the SCF calculations and observed values for He, Rb,  $\text{Rb}^+$ ,  $\text{Na}^+$ , and  $\text{Cl}^-$  : for instance, the calculated ionization potential of helium was 24.85 eV, within the difference of 0.2 eV from the observed

<sup>53</sup>Ibid., pp. 117–8.

value. He regarded this “very close agreement” as an “empirical justification of the simple approximations,” if not a “notable success of the method.”<sup>54</sup> Convinced of the usefulness of his approximation method, Hartree remarked:

It is thought that the distribution of charge in the self-consistent field is probably the best approximation to the actual distribution of charge in the atom which can be obtained without very much more elaborate theoretical and numerical work, and so is the most suitable to use in any problems involving this distribution of charge; also it is hoped that when the time is ripe for the practical evaluation of the exact solution of the many-electron problem, the self-consistent fields calculated by the methods given here may be helpful as providing first approximations.<sup>55</sup>

### Hartree’s Self-Consistent-Field Method and Slater’s Determinantal Method

Only a few months after the publication of Hartree’s papers in 1928, J. A. Gaunt of Trinity College offered a critical review of his SCF method.<sup>56</sup> Gaunt’s purpose was not to disprove the method, but to assess Hartree’s assumptions in the light of recent developments of quantum mechanics. He saw the assumptions as “simple and picturesque,” and “open to several objections” from a rigorous point of view. He particularly raised a question as to whether it was really justifiable to describe the many-electron atom as the simple product of one-electron wave functions of individual electrons, rather than as one complete wave function. This was the fundamental assumption that Hartree himself did not doubt seriously; Hartree did not even consider the Pauli exclusion principle, the spin state of electrons, or Heisenberg’s resonance phenomenon, in dealing with many-electron systems. Hartree’s method was flawed in this regard. Investigating the error possibly caused by the neglect of resonance terms, however, Gaunt showed that the terms responsible for resonance were small enough. Indeed, he found that Hartree’s method gave a better result for helium’s ionization potential than the perturbation method. Thus he concluded: “Hartree’s wave functions have been shown to be good approximations.”

A more thorough review of Hartree’s papers came from John C. Slater of Harvard University.<sup>57</sup> Like Gaunt, Slater stressed that Hartree should have considered the resonance interactions between electrons in his approximation. In addition, Slater pointed out, Hartree also neglected the fact that electron distributions were not really spherical. This was in fact what Hartree had been most concerned about. He had been aware that except for an electron of  $s$  orbit (where the azimuthal quantum number  $l = 0$ ) the electron’s own contribution to the field was not centrally symmetrical; and thus that the assumption of a central field had no general applicability. “It was just here,” Hartree had admitted, “that we meet the most serious doubts concerning the replacement of the actual many-body problem by a one-body problem with a central field for each electron, even as a first approximation.”<sup>58</sup> Besides, Slater found an inconsistency in Hartree’s

---

<sup>54</sup>Ibid., p. 117.

<sup>55</sup>Ibid., p. 114.

<sup>56</sup>J. A. Gaunt, “A Theory of Hartree’s Atomic Fields,” *Proceedings of the Cambridge Philosophical Society*, **24** (1928), 328–42.

<sup>57</sup>John C. Slater, “The Self Consistent Field and the Structure of Atoms,” *Physical Review*, **32** (1928), 339–48.

<sup>58</sup>Hartree, “Wave Mechanics. Part II,” p. 112.



method of dealing with the core (inner-shell) electrons and the valence electron: for the valence electron, he solved the problem of the core electrons first and used the central field determined from it, thus neglecting the influence of the valence electron on the core electrons. In other words, Hartree neglected the possible polarization of the inner shell by the valence electron.<sup>59</sup>

Slater's criticism was not geared toward invalidating the SCF method. Instead, by estimating the errors in it, Slater sought to provide a theoretical justification for Hartree's approximation method. Thus his conclusion was not much different from Gaunt's: "we see that none of the corrections to Hartree's terms are really much larger than the order of magnitude of his discrepancies from experiment, so that his good agreement with observation is justified."<sup>60</sup> Hoping that Hartree would not misinterpret his criticism, Slater sent him a draft of his paper. In reply, Hartree wrote: "I certainly hope you will publish this paper. . . . Certainly I do not feel at all that you are treading on my toes in working on this subject; on the contrary I am very glad the problem has attracted you, and that you and Gaunt have been able to justify the procedure I adopted empirically. If you want to do any further work involving numerical values, I would be glad to send you any numerical data I possess."<sup>61</sup>

Slater gave a critical review of the SCF method in 1928, when his main interest moved from the radiation problem to the theory of matter—atoms, molecules, and metals.<sup>62</sup> Slater sought to find out the proper ways of incorporating Pauli's exclusion principle into the problem of many-electron atoms, as Heisenberg had done for helium with the concept of resonance. In fact, many competent theoretical physicists, such as Eugene Wigner, Frederick Hund, Herman Weyl, and Walter Heitler, had been engaged in this problem since the publication of Heisenberg's helium paper in 1926. They followed the procedure Heisenberg had prescribed: first, they tried to find the appropriate form of wave functions of the ordinary position coordinates  $(x, y, z)$ , and then considered the spin needed to make the whole wave function antisymmetric with respect to the change of electrons. To this end, they used group theory. In contrast, Slater took the opposite tack, by introducing the spin at the very beginning of the calculation. This led to a much simpler way of representing the antisymmetric wave function, now known as the determinantal method, than by group theory.<sup>63</sup>

In the development of the determinantal method, Slater owed much to Hartree. For

---

<sup>59</sup>Slater, "Self Consistent Field," pp. 346–8.

<sup>60</sup>Ibid., p. 348.

<sup>61</sup>Hartree to Slater, 6 July 1928, D. R. Hartree, #1, John C. Slater Papers, American Philosophical Society, Philadelphia.

<sup>62</sup>Slater took his doctoral degree at Harvard University in 1923 under the supervision of the experimental physicist Percy W. Bridgman, writing a thesis on the compressibility of alkali halide crystals of the sodium chloride type. So it is possible to see that Slater moved back to his earlier interest. But he also felt that he was outpaced by Dirac who published a paper on quantum electrodynamics that was far more comprehensive and thorough than Slater's ideas. Paul A. M. Dirac, "The Quantum Theory of the Emission and Absorption of Radiation," *Proceedings of the Royal Society*, **A114** (1927): 243–65. Slater later wrote that after reading Dirac's paper, "It was obvious that I would never catch up with Dirac to the point of being clearly ahead of him. Thus at this point I shifted my interest to the helium atom." Quoted in Silvan S. Schweber, "The Young John Clarke Slater and the Development of Quantum Chemistry," *Historical Studies in the Physical and Biological Sciences* **20** (1990): 339–406, at p. 373. In footnote 94, Schweber has pointed out that Slater tried again and again but in vain to unify the quantum theory of radiation with that of matter.

<sup>63</sup>John C. Slater, "The Theory of Complex Spectra," *Physical Review* **34** (1929): 1293–322.

Slater profited from the analysis of Hartree's papers, from which he learned that the assumption of the central field in many-electron atoms worked out well, and that the one-electron approximation might be a good starting point even if resonance was neglected. Therefore, Slater adopted the assumption of the central field, with a slight modification for simplicity in description: "according to [Hartree's scheme], each electron moves in a field of force slightly different from the others. We shall neglect the difference, assuming that all the electrons move in precisely the same field. And this field is to be so chosen as to give the best agreement with the correct values even without further corrections."<sup>64</sup> Slater then used the one-electron approximation, representing each electron's wave function with both the position and spin coordinates. As Slater acknowledged, the process of building up the antisymmetric wave function with a determinant was well known.<sup>65</sup> What was new in his method was to represent each electron's wave function with the position and spin coordinates together, and to construct the antisymmetric wave function as the linear combination of the one-electron approximations. Slater's previous study of Hartree's one-electron approximation provided him with the confidence that this kind of approximation would lead to a good result. And he demonstrated the validity of his method by using it in the wave-mechanical study of complex atomic spectra, most notably the theoretical explanation of Hund's empirical rule for classifying spectra.

Slater sent his paper "The Theory of Complex Spectra" to the *Physical Review*, shortly before he took a trip to Europe in the summer of 1929 as a Guggenheim Fellow. Everyone he met seemed to know of his work, and most liked it. "No other work I have done," Slater wrote in his autobiography, "was so universally popular."<sup>66</sup> This paper was particularly welcomed by those physicists who saw group theory as an arcane, incomprehensible mathematical manipulation: Slater later heard such remarks as "Slater had slain the 'Gruppenpest' [the pest of group theory]." He met Hartree at a conference in Zurich, before going to Leipzig to spend half a year with Heisenberg and Hund.

While in Leipzig, Slater found that Hartree's Self-Consistent-Field method was not well received among the quantum theorists. Despite some theoretical justifications made by Gaunt and Slater, many still considered the SCF method to "stand apart from the main current of quantum theory" and "to contain arbitrary and empirical elements." Thus Slater sent a short note to the *Physical Review* in defense of the SCF method.<sup>67</sup> This time he insisted upon its close relation to the procedure a scientist should take when applying the variation principle to the simple product of one-electron wave functions. He said:

Suppose one sets up an approximate wave function for a general problem of the motion of electrons among stationary nuclei, by assuming a product of functions of the various electrons:  $u = u_1(x_1) \dots u(x_n)$ ; suppose further that one apply the variation principle by varying separately each of the functions

---

<sup>64</sup>Ibid., 1299.

<sup>65</sup>Ibid., 1294. Slater mentioned Dirac's earlier papers and the recent paper by Iva Waller and Douglas R. Hartree's "The Intensity of Total Scattering of X-rays," *Proceedings of the Royal Society* **A124** (1929): 119–42.

<sup>66</sup>Slater, *Solid-State and Molecular Theory*, 62–3. Slater noted the responses from Hund, Waller, Hartree, Bloch, Heisenberg, and Wigner. See also Schweber, "John Clarke Slater," 377.

<sup>67</sup>John C. Slater, "Note on Hartree's Method," *Physical Review* **35** (1930): 210–1.

$u_i$ , leaving the others constant. The  $n$  variation equations so obtained prove to be those for the motion of the  $n$  electrons, each in a separate electrostatic field; and the field for each electron is obtained by adding the densities  $u_i^2$  for all the other electrons, and finding by electrostatics the field of this charge and of the nuclei. Thus this field is self-consistent in the sense of Hartree; the result is a generalization of his method to more complicated problems than atomic ones.<sup>68</sup>

The variation scheme was designed to find the “best” approximate wave function by varying arbitrary parameters or arbitrary functions so that the energy of the system was stationary with respect to slight variations of them. Slater realized that this way of finding the “best” approximate wave function was tantamount to that of finding the “self-consistent” field: that is, the “best” function would lead to the “self-consistent” field, or vice versa. One notable difference in practice was that the variation procedure did not include the spherical averaging of potential. Hartree needed this step to compare the initial and final fields in terms of the actual charge distributions of those fields; but in the variation procedure, the comparison was made as to the convergence of the energy in the successive variations of the initial trial wave function.

In his note, Slater also hinted that the exclusion principle could be considered in the SCF method by using his determinantal representation of the antisymmetric function. Yet he did not show there how to set up an elaborate formulation of applying the variation principle to the antisymmetric function. A few months later, the Russian physicist Vladimir Fock developed another way of formulating the SCF method with the variation principle. Unfamiliar with Slater’s determinantal method, Fock used the technique of the permutation group.<sup>69</sup> Hence the Hartree-Fock (instead of the Hartree-Slater-Fock) method. In 1935, finally, Hartree simplified Fock’s formulation with Slater’s determinantal method.<sup>70</sup>

The Hartree-Fock method was universally accepted, not because it produced results as accurate as Hylleraas had achieved with helium, but because it provided a manageable tool for handling heavy atoms. From the beginning, it was realized that this method was only of limited accuracy, giving errors of around 1 percent. The source of the errors was also well known: the neglect of electron correlation. Hartree’s original SCF method presumed that electrons moved completely independently of each other; and Fock’s elaboration remedied this problem partially, only through the requirement of antisymmetry of wave function. This kind of electron correlation was regarded as “accidental,” since it stemmed from the Pauli principle rather than from the electrostatic requirement that the electrons should keep away from one another. The further refinement of the Hartree-Fock method was thus made to consider electron correlation in a more general way.<sup>71</sup> Despite this problem, there was a consensus that Hartree-Fock ap-

---

<sup>68</sup>Ibid., 211.

<sup>69</sup>Vladimir Fock, “Näherungsmethode zur Lösung des quantenmechanischen Mehrkörperproblems,” *Zeitschrift für Physik* **61** (1930): 126–48. This paper was received on 21 February 1930. In it, Fock did not mention any of Slater’s work; but he cited Gaunt’s paper on Hartree’s method.

<sup>70</sup>Douglas R. Hartree and William Hartree, “Self-Consistent Field, with Exchange, for Beryllium,” *Proceedings of the Royal Society* **A150** (1935): 9–33. See also, Douglas R. Hartree, “Theory of Complex Atoms,” *Nature* **138** (1936): 1080–82.

<sup>71</sup>For the source of the errors in the SCF method, see Frederick Seitz, *The Modern Theory of Solids* (New York: McGraw-Hill, 1940), 237. See also Slater, “Hartree-Fock Method,” 480.

proximations were the “best possible” one-electron wave functions, and that these were “the only wave functions which can be used in most problems concerning the energy levels of complex systems.”<sup>72</sup>

Although the idea of the self-consistent-field was the central part of Hartree’s original method or its modified form, Hartree’s genius lay in his numerical analysis of difficult wave equations. For each cycle of approximations, and for each of the electrons in atoms, he had to solve the differential equation of radial function, which could not be done analytically. So Hartree developed a technique of numerical integration, basically a way of solving the equation at numerous fixed points of  $r$ , the distance from the nucleus; and computations took up so much of his energy that he failed to keep abreast of the recent development of quantum theory. In reply to Slater’s criticism in 1928, he said: “Some of the steps were not clear to me without a bit of work and looking up the general theory, but that is my fault; my time has been so taken up with the development of the numerical technique of evaluating the self-consistent field, and with the actual computing of particular cases, that I am not as familiar as I should be with the general theory outside what I have required for my work, which is not much.”<sup>73</sup> In the 1930s Hartree was fortunate to have the assistance of his father, William Hartree, who liked doing the computing work as an occupation for his retirement.<sup>74</sup> Hartree also looked for computing machines to relieve the amount of human labor. In the early 1930s, he visited MIT to learn about Vannevar Bush’s differential analyzer<sup>75</sup>; and on his return to Britain, he set up his own model of a differential analyzer with Meccano parts (children’s toys) to demonstrate its working. After World War II, he again made a trip to America to become familiar with the ENIAC (Electronic Numerical Integrator and Computer), the electronic digital computer built for the purpose of calculating the trajectories of projectiles during the war. On his return, Hartree published more than a dozen very detailed reports on this machine for the general public as well as for the scientific community, and lent his expertise to the installation of digital computers in England, including the EDSAC (Electronic Discrete Variable Automatic Computer) in Cambridge and the Ferranti in Manchester. The popularization of computers and their application to scientific problems became his major activity for several years after his return to Cambridge in 1946, when he succeeded Fowler as Plummer Professor of Mathematical Physics. It is no surprise that the title of his inaugural lecture was “Calculating Machines, Recent and Prospective Developments.”<sup>76</sup>

---

<sup>72</sup>Eyring et al., *Quantum Chemistry*, 166.

<sup>73</sup>Hartree to Slater, 6 July 1928, D. R. Hartree #1, John C. Slater Papers, American Philosophical Society, Philadelphia.

<sup>74</sup>In 1939, Hartree wrote to Slater: “As you may know, all the computing work in the calculations of atomic structures which my father and I have published during the last several years has been done by him. He likes it as an occupation for his retirement, and I am glad to have his help, as I would not have the time to carry through the rather extensive computations myself.” Hartree to Slater, 1 November 1939, D. R. Hartree, #1, John C. Slater Papers, American Philosophical Society, Philadelphia.

<sup>75</sup>Perhaps it was Slater who provoked Hartree to pay a visit to MIT. In his letter to Hartree on 25 November 1931, Slater gave a description of Bush’s differential analyzer, and said he planned to use this machine in the SCF calculations. D. R. Hartree, #1, John C. Slater Papers, American Philosophical Society, Philadelphia.

<sup>76</sup>Douglas R. Hartree, *Calculating Machines, Recent and Prospective Developments* (Cambridge: Cambridge University Press, 1947). Thirteen out of forty publications by Hartree after 1946 were intended to inform the readers of various journals and governmental officials about calculating machines. For the bibliography of Hartree’s work, see C. G. Darwin, “Douglas Rayner Hartree,” pp. 112–6. For

## Computations in the History of Quantum Theory

Hartree's deep interest in improving calculation techniques and easing human labor did not earn him much respect among quantum physicists. Slater found it unfair. He said: "Douglas Hartree was very distinctly of the matter-of-fact habit of thought that I found most congenial. The hand-waving magical type of scientist regarded him as a 'mere computer.' Yet he made a much greater contribution to our knowledge of the behavior of real atoms than most of them did."<sup>77</sup> Slater went on to argue that Hartree's contributions should be seen in a broader context: "while he limited himself to atoms, his demonstration of the power of the self-consistent field for atoms is what has led to the development of that method for molecules and solids as well." Indeed, a convenient method of dealing with molecular problems was developed in the early 1950s by adapting the procedure of the self-consistent field approximation.<sup>78</sup>

Yet Hartree was not alone in having to cope with the prejudice against computation-oriented research. Sugiura's work failed to impress even Heitler, who said: "It appears that there are in the world some hard working dwarfs" said Heitler, who put more value on gaining physical explanations than having exact computations.<sup>79</sup> Heitler's attitude was not much different from Heisenberg's. After finishing his path-breaking paper on helium, Heisenberg remarked: "I am convinced that the spectra of all chemical elements can be obtained . . . from quantum mechanics in a unique manner without physics [i.e., physical insights] by bone-headed calculation."<sup>80</sup>

To a large extent, the historical significance of computation in quantum mechanics has been undervalued or unexplored. How much, then, do we have to pay attention to those "hard working dwarfs" or "bone-headed" computers? Where is their proper place in the history of quantum physics and chemistry? As long as we confine ourselves to the "conceptual" development of quantum mechanics, it will be difficult to find answers to these questions. A clue may be in the "practice" of theory to make its incremental improvement or circumvent technological or even conceptual constraints. In this respect, the following two recollections are illustrative. Heitler recalled his Eureka moment:

I slept till very late in the morning, found I couldn't do work at all, had a quick lunch, went to sleep again in the afternoon and slept until five o'clock. When I woke up . . . I had clearly . . . the picture before me of the two wave functions of two hydrogen molecules joined together with a plus and minus

---

Hartree's role in the introduction of computers in England, see Mary G. Croarken, "The Emergence of Computing Science Research and Teaching at Cambridge, 1936–1949," *Annals of the History of Computing*, **14** (1992), 10–15; Paul A. Medwick, "Douglas Hartree and Early Computations in Quantum Mechanics," *Annals of the History of Computing*, **10** (1988), 105–11.

<sup>77</sup> Slater, *Solid-State and Molecular Theory*, p. 54. Slater held that there were two quite different types of thinkers among theoretical physicists. "One type is the prosaic, pragmatic, matter-of-fact sort, who indicates the argument behind what he does, and tries to write or speak in the most comprehensible manner possible. The other is what we might call the magical or hand-waving type, who like a magician, waves his hands as if he were drawing a rabbit out of a hat, and who is not satisfied unless he can mystify his readers or hearers." He believed that Heisenberg and Schrödinger, as well as Hartree, belonged to the first group; and that Dirac was definitely among the second group. See *ibid.*, p. 42.

<sup>78</sup> Clemens C. J. Roothaan, "New Developments in Molecular Orbital Theory." *Reviews of Modern Physics*, **23** (1951), 61–89.

<sup>79</sup> Quoted in Gavroglu, *Fritz London*, p. 47.

<sup>80</sup> Werner Heisenberg to Pascual Jordan, 28 July 1926, quoted in Mehra and Rechenberg, *The Formulation of Matrix Mechanics and Its Modifications*, p. 301.

and with the exchange in it. So I was very excited, and I got up and thought it out. As soon as I was clear that the exchange did play a role, I called London up, and he came to me as quickly as possible. Meanwhile I had already started developing a sort of perturbation theory. We worked together then until rather late at night, and then by that time most of the paper was clear. . . . Well, . . . at least it was not later than the following day that we had the formation of the hydrogen molecule in our hands, and we also knew that there was a second mode of interaction which meant repulsion between two hydrogen atoms—also new at the time—new to chemists, too.<sup>81</sup>

Heitler and London may have finished essential parts of their paper almost overnight. By contrast, a widely circulated rumor had it that James and Coolidge spent three years on the hydrogen problem, although, in fact, it took about half a year. But had they had no previous experience of computations with  $Li_2$ ,  $Cl_2$ , and  $H_2O$ , it would certainly have taken longer than that. James later said:

The idea of applying to  $H_2$  a treatment analogous to that of the helium atom by Hylleraas came to me in the bathtub—in keeping with the tradition of Archimedes, but with less evident relevance. I made some general notes on the project while I was at home, but I did not have facilities there to begin the calculation. I was familiar enough with molecular calculations to realize how much labor would be involved, and my earlier cooperation with Coolidge had made evident the great advantages of collaboration in such complex numerical calculations. When I returned to Cambridge in the fall of 1932 I discussed with Professor Kemble the possibility of undertaking this project in collaboration with Coolidge.<sup>82</sup>

Working with machines that seem primitive from today's standpoint (they started with hand-powered desk calculators and later used motor-driven ones), they found it delightful to get good results after their labor-intensive calculations. "I remember," James said, "as among the happiest and most exciting days of my life the period in which we saw the numerical results come out better and better as we added more and more terms to our calculation."<sup>83</sup> James's Eureka moment came with the realization that enormous labor would be required to proceed his idea, and his rewarding moment came when the theoretical values came closer to experimental ones.

Shortly after the advent of quantum mechanics, several ways of solving the many-electron Schrödinger equation were developed, but there were considerable difficulties in carrying out these solutions. As Per-Olov Löwdin, a Swedish quantum chemist, quipped in the 1950s: "It is sometimes said that a theoretician is a person who knows how to solve a problem, but who cannot do it."<sup>84</sup> Sugiura, James, Hartree, and other *ab initio*ists were those who did it. To them, making a theory really work in atomic and molecular

---

<sup>81</sup>Walter Heitler, AHQP (Archive for the History of Quantum Physics) Interview, pp. 541–542, Historical Development of Quantum Theory, volume 6. 1963.

<sup>82</sup>James to Sopka, 9 May 1972, quoted in Sopka, *Quantum Physics*, pp. 4.87–4.88.

<sup>83</sup>Ibid., p. 4.88.

<sup>84</sup>Per-Olov Löwdin, "Recent Simplifications in the Molecular Orbital Theory of Calculating Energy Levels," in *Proceedings of the International Conference of Theoretical Physics* (Tokyo: Nippon Bunka Insatsusha Co., 1953), 599–609, quote on 599.

problems was as important as developing it in the first place. Computational imperatives in the early years of quantum chemistry clearly reveal the emerging practice of theory that required human labor, technological improvement (computers), and mathematical ingenuity. In no small measure, this practice contributed to demonstrating the validity of quantum mechanics and its usefulness.

# 17 A Service for the Physicists? B. L. van der Waerden's Early Contributions to Quantum Mechanics

MARTINA R. SCHNEIDER

Bartel Leendert van der Waerden (1903–1996) was a scientist with a wide range of interests. He contributed to invariant theory, algebraic geometry, algebra, topology, statistics and probability theory, as well as to physics and to the history of mathematics, astronomy and physics. In this paper<sup>1</sup> I will try to characterize his early contributions to quantum mechanics which he wrote around 1930.<sup>2</sup> All of these deal with group theory, a mathematical theory which was well established at the time but whose application to quantum mechanics was quite controversial. How did van der Waerden come to publish something in this field? What kind of mathematics did he use? What was his stance in the debate about the “group plague”?

In order to give an idea in which direction these questions might be answered three examples from his papers will be discussed. These examples concern van der Waerden's development of the spinor calculus, his introduction to representation theory by a concept called group with operators, and his treatment of Slater's method, a method which explicitly was aimed at avoiding group theory. Local networks (in Göttingen, the Netherlands and Leipzig) which were a stimulus for van der Waerden's work in physics and, to some extent, had an influence on the direction of his research are sketched. By comparing van der Waerden's approach to that of H. Weyl and E. Wigner, two main advocates of the group-theoretic method in quantum mechanics at the time, some of its characteristic features are revealed and the wider (scientific) context is brought into the analysis. Finally, an attempt is made to answer the question of the title with respect to the discussed examples.

---

<sup>1</sup>I dedicate this article to Erhard Scholz on the occasion of his 60th birthday. A more detailed analysis of van der Waerden's early contributions to quantum mechanics will be given in my PhD thesis “Die physikalischen Beiträge des jungen Bartel Leendert van der Waerden” (Wuppertal, to appear 2008).

<sup>2</sup>van der Waerden [1929, 1932]; Infeld and van der Waerden [1933]. For a list of his publications see Top and Walling [1994]. Despite its impressive length it is still incomplete.



## Background

Van der Waerden<sup>3</sup> studied mathematics and physics with H. de Vries, G. Mannoury, R. Weitzenböck, L. E. J. Brouwer and J. D. van der Waals jr. at Amsterdam university between 1919 and 1924. In autumn 1924 he went to Göttingen on a Rockefeller grant. There he studied for one year with E. Noether, R. Courant and D. Hilbert. During this stay van der Waerden got to know the new methods of modern algebra developed by Noether and E. Artin and others and which he applied to give a better foundation of the Schubert calculus in his thesis. Although van der Waerden had done physics in Amsterdam, according to his own account it was in Göttingen where he studied mathematical physics in 1924 and read Courant and Hilbert's recent book on the methods of mathematical physics, and was deeply impressed by it.<sup>4</sup> Brouwer had given him a letter of recommendation for Courant and van der Waerden was soon drawn into Courant's small working unit on mathematical physics consisting of K. O. Friedrichs, H. Lewy and P. Jordan. Van der Waerden left Göttingen in 1925 to do his military service in the Netherlands and to write his PhD thesis. Then, in summer 1926, he went to Hamburg on the rest of his Rockefeller grant where he continued to study modern algebra with Artin. When the grant ran out he got a position as assistant to H. Blaschke in Hamburg. So, van der Waerden was not in Göttingen, but in the Netherlands and in Hamburg when W. Heisenberg, M. Born and Jordan developed matrix mechanics.

In spring 1927 he returned to Göttingen where he worked as an assistant for Courant. He wrote his habilitation on Bézout's theorem. In 1928 he got his first professorship in Groningen in the Netherlands. As we will see, his time in Groningen was quite important for the development of his first work on quantum theory. He returned as a visiting professor to Göttingen in summer 1929. In 1930/31 he published a text book on modern algebra which was based on the lectures of Noether and Artin. It quickly became a bestseller. In May, 1931, van der Waerden was appointed professor in Leipzig. He was especially looking forward to going there because Heisenberg and F. Hund were there too.<sup>5</sup> In fact, he regularly attended their seminar on the structure of matter. In the winter term 1931/32 he gave a course of lectures on group-theoretic methods in quantum mechanics. He also proposed and supervised the PhD thesis of H. A. Jahn on the rotation and oscillation of the methane molecule which included the Jahn-Teller effect.<sup>6</sup> It was in Groningen and Leipzig where he wrote the papers on quantum mechanics from which the examples for this analysis are taken.

Van der Waerden published several works on physics.<sup>7</sup> His first publication at the

---

<sup>3</sup>For information on van der Waerden's biography see Gross [1973]; Eisenreich [1981]; van der Waerden [1983]; Frei [1993]; Freit et al. [1994]; Dold-Samplonius [1994]; Scriba [1996a,b]; Dold-Samplonius [1997]; Frei [1998]; Thiele [2004]; Soifer [2004a,b, 2005]. There is no scientific biography to date. A first step in this direction is a paper by Schappacher [2003] on van der Waerden's early contributions to the development of algebraic geometry. The photo of van der Waerden (Figure 1) is taken from the photo collection Veenhuijzen, Centraal Bureau voor Genealogie (Den Haag).

<sup>4</sup>Courant and Hilbert [1924].

<sup>5</sup>For information on the physics department in Leipzig during Heisenberg's professorship see e. g. Kleint and Wiemers [1993], on the interrelationship between mathematics and physics in Leipzig see Schlote [2007].

<sup>6</sup>Jahn [1935].

<sup>7</sup>van der Waerden [1921, 1929, 1932]; Infeld and van der Waerden [1933]; van der Waerden [1941, 1963, 1966, 1975]. He also contributed to the history of quantum mechanics [van der Waerden 1960, 1967,



Figure 17.1: Bartel Leendert van der Waerden, Groningen 1928

age of 18 was a popular account of special and general relativity theory based on a lecture given by P. Ehrenfest.<sup>8</sup> Several years later he published three works on quantum mechanics, one along with L. Infeld. Van der Waerden developed a spinor calculus in special and general relativity theory and applied it to the wave equation of the electron<sup>9</sup> and he wrote a monograph on the group-theoretic method in quantum mechanics<sup>10</sup>. This monograph was the last in a row of three books on the same subject. In 1931 both Wigner and Weyl had published monographs, too.<sup>11</sup> In the case of Weyl, this was the second, revised edition of his comprehensive book from 1928. When van der Waerden learned of Wigner's publication he almost withdrew from his project. It was Courant who convinced him to carry on.<sup>12</sup>

Group theory had been introduced into quantum mechanics in 1926/27 by Heisenberg, Wigner, J. von Neumann and Weyl.<sup>13</sup> With the help of this new method one was able to mathematically deduce the quantum numbers (except for the quantum number  $n$ )

---

1973, 1976].

<sup>8</sup>van der Waerden [1921].

<sup>9</sup>van der Waerden [1929]; Infeld and van der Waerden [1933].

<sup>10</sup>van der Waerden [1932].

<sup>11</sup>Wigner [1931]; Weyl [1977].

<sup>12</sup>I thank Volker Remmert for this piece of information.

<sup>13</sup>For information on the history of the group-theoretic method in quantum mechanics see Mackey [1988a,b]; Sigurdsson[1991], Mehra and Rechenberg [chap. III.4(e) 2000], Chayut [2001]; Scholz [2006] and the contributions of E. Scholz and C. Smeenk in this volume.

which had been based on an empirical analysis of spectra of atoms and molecules. The algebraically simple structures of irreducible representations (of the group of rotations and of the group of permutations) could be directly related to quantum numbers. Moreover, Wigner and Weyl also explored the conceptual power of group theory for the foundation of quantum mechanics. W. Heitler and F. London applied group-theoretic methods to explain the binding of atoms. The method, however, was met with resistance by a lot of physicists and chemists, mainly because they were not acquainted with group theory and found it difficult to learn. There was also a feeling that group-theoretic reasoning was essentially “not physical” (nicht physikalisch).<sup>14</sup> The term “group plague” (Gruppenpest) was coined. It was within this context that van der Waerden entered quantum mechanics.

## Spinor Calculus—a Calculus on Demand

Van der Waerden developed spinor calculus in Groningen. He did so at the request of Ehrenfest in Leiden in spring 1929. Ehrenfest’s question dates back to autumn 1928 when he tried to get a grip on group-theoretic methods in order to understand the works of Weyl, Wigner and von Neumann. Ehrenfest organized a series of lectures inviting specialists like Wigner, W. Pauli, Heitler, London and von Neumann. He also invited van der Waerden who had just got his first professorship in Groningen. Ehrenfest used van der Waerden as a kind of mathematical advisor:

I [Ehrenfest] would like to ask you [van der Waerden] about various mathematical things, very basic for you, because unfortunately a real group plague [Gruppenpest] has broken out in our physical journals. Almost all of my questions will refer to certain places in Weyl’s new book: “Gruppentheorie und Quantenmechanik”, and in it mainly to the different “integer and half-integer” representations of the rotation group in three- and four-dimensional space.<sup>15</sup> [Ehrenfest to van der Waerden, 8.10.1928]

Van der Waerden was drawn into a Dutch circle of physicists by Ehrenfest, a circle consisting mainly of Ehrenfest’s students and former students like H. Kramers, G. Uhlenbeck, S. Goudsmit, D. Coster and H. B. G. Casimir.

Van der Waerden developed a formalism to handle “spinors,” a term probably coined by Ehrenfest. Spinors are quantities in representation spaces of the Lorentz group or of its subgroups. They had appeared implicitly or explicitly a couple of times in quantum mechanics: in the works of Pauli, Wigner, Weyl and P. A. M. Dirac. Van der Waerden was asked by Ehrenfest to develop a spinor calculus modelled on tensor calculus to handle these quantities more easily. So Ehrenfest had a mathematical formalism designed for calculation in mind.

---

<sup>14</sup>Wigner [1931, preface, p. V].

<sup>15</sup>“Ich [Ehrenfest] habe Sie [van der Waerden] ueber verschiedene fuer Sie ganz elementare mat[h]ematische Dinge zu fragen, da ja leider eine wahre Gruppenpest in unseren physikalischen Zeitschriften ausgebrochen ist. Fast alle meine Fragen werden sich auf bestimmte Stellen aus dem neuen Buch von Weyl: Gruppentheorie und Quantenmechanik beziehen und da wieder hauptsaechlich auf die verschiedenen ‚ganz- und halbzahligen‘ Darstellungen der Drehgruppe im Drei- und vierdimensionalen Raum.” [Museum Boerhaave in Leiden (MB), Ehrenfest Scientific Correspondence (ESC) 10, S.6, 217] The translation as well as the other translations in this paper are mine (MS).

In his article van der Waerden [1929] developed this calculus with a minimum of mathematical prerequisites: He neither touched the theory of representation, nor did he explain the theory of invariants or the underlying geometric picture. For example, he did not give a formal, let alone axiomatic definition of representation, but rather mentioned it, in passing by, in a concrete setting:

The task to find all “quantities” that are transformed linearly by the Lorentz-transformations according to any kind of rule, so that with a composition of two Lorentz-transformations the corresponding transformations of the “quantities” are combined too, i. e. so that the product of two Lorentz-transformations is expressed again by the product, is simply the problem of the *representation* of the Lorentz group through linear transformations.<sup>16</sup>  
[van der Waerden, 1929, p. 101, emphasis in the original]

This was not in line with a modern approach to representation theory of that time. It shows van der Waerden’s capability and willingness to adapt to different scientific contexts and audiences.

Van der Waerden introduced the spinor formalism by letting the special linear group of complex  $2 \times 2$  matrices ( $SL_2\mathbb{C}$ ) act on a two-dimensional complex vector space. He described the standard representation and the complex conjugate standard representation of  $SL_2\mathbb{C}$ . He did this by explicitly giving the equations for the transformed vectors. He then generalized the operation of  $SL_2\mathbb{C}$  to factors of “products” consisting of components of vectors in a two-dimensional space by factorwise operation, i.e. he described the action of  $SL_2\mathbb{C}$  on tensor products. He introduced the following notation: If  $\bar{\xi}_\lambda$  and  $\bar{\eta}_\mu$  are transformed by the complex conjugate standard representation and  $\zeta_\nu$  by the standard representation then he denoted quantities transforming like the “product”

$$\bar{\xi}_\lambda \bar{\eta}_\mu \zeta_\nu$$

of these components by the spinor

$$a_{\dot{\lambda}\dot{\mu}\nu}$$

(with  $\lambda, \mu, \nu = 1, 2$ ). These “dotted” indices are still in use today. Van der Waerden also showed in analogy to the classical tensor calculus how the indices are pulled up and down:

$$a^1 = a_2, a^2 = -a_1 \quad \text{and} \quad a^{\dot{1}} = a_2, a^{\dot{2}} = -a_1.$$

Today, this relation is denoted typically with the help of the skew-symmetric  $\epsilon$ -tensor

$$(\epsilon^{\lambda\mu}) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

as  $a^\lambda = \epsilon^{\lambda\mu} a_\mu$ .<sup>17</sup> So, van der Waerden outlined the foundations of the spinor calculus.

---

<sup>16</sup>“Die Aufgabe, alle ‚Größen‘ zu finden, die bei Lorentztransformationen nach irgendeiner Regel linear mit-transformiert werden, so daß bei Zusammensetzung zweier [!] Lorentztransformationen auch die zugehörigen Transformationen der ‚Größen‘ zusammengesetzt werden, d.h. so daß dem Produkt zweier Lorentztransformationen wieder das Produkt entspricht, ist nichts anderes als das Problem der *Darstellung* der Lorentzgruppe durch lineare Transformationen.”

<sup>17</sup>Van der Waerden introduced the  $\epsilon$ -tensor as a “pure spinor” into spinor calculus to construct invariants [van der Waerden, 1932, p. 86f].

Then van der Waerden established a 2 : 1 homomorphism between  $SL_2\mathbb{C}$  (considered as a real Lie group) and the proper orthochronous Lorentz group  $\mathcal{L}_+^\uparrow$  by giving a concrete mapping between spinors of the form  $a_{\lambda\mu}$  and the coordinates of a real four-dimensional vector space. In other words, he gave a bijection between  $2 \times 2$  Hermitian matrices and Minkowski space. Thus, one got an irreducible representation of  $SL_2\mathbb{C}$  and a “two-valued” (zweideutige) representation of  $\mathcal{L}_+^\uparrow$  where one could assign  $\pm A \in SL_2\mathbb{C}$  to one Lorentz-transformation. For his construction van der Waerden could rely on the work of Weyl on representation theory and of E. A. Weiß on invariant theory.<sup>18</sup> Thus, mathematically, it was not a great challenge.

Van der Waerden then applied this calculus to physics: he translated the relativistic Dirac wave equation into spinor formalism. He started out with a slightly modified version of this wave equation given by Weyl in his book<sup>19</sup>

$$\frac{1}{c} \left( \frac{\hbar}{i} \frac{\partial}{\partial t} + \Phi_0 \right) \psi + \sum_{r=1}^3 s'_r \left( \frac{\hbar}{i} \frac{\partial}{\partial x_r} + \Phi_r \right) \psi + mc\Gamma_0\psi = 0,$$

where the wave function  $\psi$  has four components  $\psi_i : \mathbb{R}^4 \rightarrow \mathbb{C}$ . Translating this equation step-by-step into spinor calculus he ended up with a pair of spinor equations corresponding to the first two and the last two rows of Weyl’s equation:

$$\begin{aligned} - \left( \frac{\hbar}{i} \partial_\mu^\lambda + \Phi_\mu^\lambda \right) \psi_\lambda + mc\chi_\mu &= 0 \\ \left( \frac{\hbar}{i} \partial_\mu^\lambda + \Phi_\mu^\lambda \right) \chi_\lambda + mc\psi_\mu &= 0, \end{aligned}$$

where the wave function consists of four spinor-components  $\psi = (\psi_1, \psi_2, \chi_1, \chi_2)$  that are complex-valued functions and correspond to the irreducible representations of  $SL_2\mathbb{C}$ , and  $\Phi$  is a field.

Van der Waerden did not stop there, but outlined the general spinor form of wave equations of the first order with a two-component wave-function, and of the second order with a two-component and a four-component wave function. Thus, he provided the physicists with a multitude of different forms of wave equations in spinor formalism. By doing so, he was able to answer Ehrenfest’s question why a two-component wave function together with a wave equation of the first order would not suffice to describe

<sup>18</sup>Weiß [1924]; Weyl [1925, 1926, 1931].

<sup>19</sup>van der Waerden [1929, p. 106f], Weyl [1928, p. 172]. The constant  $\hbar$  is Planck’s constant divided by  $2\pi$  (today’s notation is  $\hbar$ ),  $m$  is the mass of the electron,  $c$  the velocity of light,  $\Phi_k$  denotes the electrostatic potential and the four-by-four matrices  $s'_r$ , are built up by Pauli spin matrices  $s_r$  ( $r = 1, 2, 3$ ) as follows:

$$s'_r = \begin{pmatrix} s_r & 0 \\ 0 & -s_r \end{pmatrix}$$

with

$$s_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad s_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad s_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The four-by-four matrix  $\Gamma_0$  is of the form

$$\begin{pmatrix} 0 & E \\ E & 0 \end{pmatrix}.$$

The matrices  $s'_r$  correspond up to a change of bases to Dirac’s  $\gamma_k$ -matrices.

the electron relativistically. Van der Waerden showed that a wave equation with a two-component wave-function of the first order

$$\partial_{\lambda\mu} \psi^\mu + c_{\lambda\mu} \psi^\mu = 0,$$

would imply that the mass of the electron is zero, which rules out this possibility.<sup>20</sup> Later, Ehrenfest used this very question in Casimir's examination.<sup>21</sup> So, Ehrenfest seems to have been convinced by van der Waerden of the usefulness of spinor calculus. Later, in spring 1933, van der Waerden helped Infeld, a Polish physicist visiting Leipzig, to introduce a spinor formalism for general relativity theory in order to find an alternative to the “*n*-Bein”-formalism which Leipzig physicists preferred not to use.<sup>22</sup> This shows van der Waerden as a very pragmatic scientist who respected the wishes of his colleagues and who made an effort to adapt to their special needs.

How was the spinor calculus received by Ehrenfest and other physicists? Uhlenbeck, a former student of Ehrenfest, together with O. Laporte published an article in the *Physical Reviews*—the American journal in which Slater had had his group-free method published two years before—advocating the use of spinor calculus.<sup>23</sup> They stated the rules of the calculus very clearly and applied it to the Dirac equation as well as to the Maxwell equations. Ehrenfest, however, was still not fully satisfied. What he wanted was an easy introduction to both tensors and spinors, and he also had some more conceptual questions.<sup>24</sup> It was he who urged A. Einstein and W. Mayer to develop their alternative concept of semivectors.<sup>25</sup> Later, in 1936, the spinor calculus was used by Dirac to derive wave equations for particles with spin greater than one half, that means wave equations for (elementary) particles that had not been discovered up to then.<sup>26</sup> And it is probably this publication by this prominent researcher which made the spinor calculus known to a wider audience and ensured that it was not forgotten.

## Modern Representation Theory: Groups with Operators

The next example will show that van der Waerden did not refrain from using modern algebraic concepts and methods in his group-theoretic monograph on quantum mechanics.<sup>27</sup> His introduction to representation theory was based on the concept “group with operators”, a concept that had not appeared in any of the other articles or books on

---

<sup>20</sup>The correspondence between Ehrenfest and van der Waerden shows that van der Waerden started out with a different equation. The published equation corresponds to Weyl's equation [Weyl, 1929, p. 351] which van der Waerden may have come across in Göttingen in summer 1929. It was later used by Pauli to describe the neutrino.

<sup>21</sup>Ehrenfest to Uhlenbeck, 1.6.1930 [MB, ESC 10, S.2, 78].

<sup>22</sup>Van der Waerden to Schouten, 6.6.1933 [Centrum voor Wiskunde en Informatica (Amsterdam), correspondence Schouten. I thank Gerard Alberts for drawing my attention to this archive.] On the history of unified field theory see Goenner [2004].

<sup>23</sup>Laporte and Uhlenbeck [1931].

<sup>24</sup>Ehrenfest [1932].

<sup>25</sup>van Dongen [2004].

<sup>26</sup>Dirac [1936]. The elementary particles electron, positron, neutron, proton, known at that time, all had spin one half. However, from 1928 onwards it was known that the nitrogen nucleus had spin one by precision measurements performed by R. de Laer Kronig in Utrecht.

<sup>27</sup>van der Waerden [1932, chap. 2].

group-theoretic methods in quantum mechanics before. So, van der Waerden's approach was unique in this respect.

The concept "group with operators" was first introduced in 1925 by W. Krull.<sup>28</sup> Krull had used a different name for it: generalized finite abelian group (verallgemeinerte endliche Abelsche Gruppe). O. Schmidt and Noether took up the concept and made it more general.<sup>29</sup> It was Noether who introduced the name "group with operators" in a very general setting. Van der Waerden also used the concept in his book on modern algebra.<sup>30</sup>

In his introduction to group theory in his monograph on quantum mechanics van der Waerden made use of the concept group with operators only in the restricted sense introduced by Krull. His definition went as follows. Van der Waerden firstly defined a group. The definition he gave there was axiomatic and general and thus in line with modern algebra<sup>31</sup>:

A set  $\mathfrak{g}$  of *elements*  $a, b, \dots$  of any kind (e.g. of numbers, of linear transformations) is called a *group* if the following four conditions are satisfied:

- (8.1.) A "product"  $a \cdot b$  (or  $ab$ ) is assigned to each pair of elements  $a, b$  in such a way that it belongs again to  $\mathfrak{g}$ .
- (8.2.) The law of associativity  $ab \cdot c = a \cdot bc$ .
- (8.3.) There exists a "unit element",  $e$  or  $1$ , with the property  $ae = ea = a$ .
- (8.4.) For each  $a$  of  $\mathfrak{g}$  there exists an inverse  $a^{-1}$  in  $\mathfrak{g}$ , so that  $a \cdot a^{-1} = a^{-1} \cdot a = 1$  holds.

The group is called *abelian*, if  $ab = ba$  always applies.

[...] Generally one speaks of a *group with operators* if certain "multipliers" or "operators"  $\theta$  with the property (8.5) [i.e.

$$\theta(u + v) = \theta u + \theta v \quad (u, v \in \mathfrak{g})]$$

are added to an abelian group.<sup>32</sup>

[van der Waerden, 1932, p. 28f, emphasis in the original]

Notice that there are very few restrictions on the set of operators.

Van der Waerden applied the concept of group with operators to the representation space. The representation space is a vector space, thus its vectors form an abelian group with respect to addition. The set of operators are the scalars together with the

---

<sup>28</sup>Krull [1925, 1926].

<sup>29</sup>Noether [1927]; Schmidt [1928]; Noether [1929].

<sup>30</sup>van der Waerden [1930, 1931].

<sup>31</sup>On the development of modern algebra see e. g. Corry [1996].

<sup>32</sup>„Eine Menge  $\mathfrak{g}$  von *Elementen*  $a, b, \dots$  irgendwelcher Art (z.B. von Zahlen, von linearen Transformationen) heißt eine *Gruppe*, wenn folgende vier Bedingungen erfüllt sind:

- (8.1.) Jedem Elementenpaar  $a, b$  ist ein „Produkt“  $a \cdot b$  (oder  $ab$ ), das wieder zu  $\mathfrak{g}$  gehört, zugeordnet.
- (8.2.) Das Assoziativgesetz:  $ab \cdot c = a \cdot bc$ .
- (8.3.) Es gibt ein „Einselement“,  $e$  oder  $1$ , mit der Eigenschaft  $ae = ea = a$ .
- (8.4.) Zu jedem  $a$  von  $\mathfrak{g}$  existiert ein Inverses  $a^{-1}$  in  $\mathfrak{g}$ , so daß  $a \cdot a^{-1} = a^{-1} \cdot a = 1$  ist.

Die Gruppe heißt *Abelsch*, wenn stets  $ab = ba$  ist. [...] Man redet im allgemeinen, wenn zu einer additiven [d. i. Abelschen] Gruppe gewisse „Multiplikatoren“ oder „Operatoren“  $\theta$  mit der Eigenschaft (8.5.) [d. i.  $\theta(u + v) = \theta u + \theta v$ ] hinzugenommen werden, von einer *Gruppe mit Operatoren*.“

representation matrices of the group in question. This makes the representation space into a group with operators. Van der Waerden showed how the central concepts of representation theory, such as invariant subspaces or irreducible representation, can be deduced from the theory of groups with operators.

One advantage of groups with operators was that van der Waerden could easily prove an important uniqueness theorem: If a representation splits into irreducible representations then this splitting is unique up to isomorphism. This was a central theorem of representation theory. It was also vital for quantum mechanics because of the correspondence between irreducible representations and quantum numbers. Proving the uniqueness theorem was elementary in this general setting.<sup>33</sup>

Wigner and Weyl also mentioned this central theorem of group theory. Wigner maintained it in full generality, but only proved it for groups with a finite number of elements.<sup>34</sup> He used so-called transcendental methods relying on characters. This approach went back to G. Frobenius and I. Schur.<sup>35</sup> It had the advantage of achieving a constructive method for reducing a given representation into irreducibles. This was also how Weyl had proceeded in the first edition of his book. However, in the second edition he changed to a more modern approach.<sup>36</sup> Although he did not introduce the concept of group with operators he used it implicitly. Weyl thought that this approach was more elementary and that it allowed a “full insight” (*vollen Einblick*) into the situation and a “complete understanding of the context” (*restloses Verständnis der Zusammenhänge*).<sup>37</sup>

Van der Waerden also saw another advantage of the concept of groups with operators, especially in physical contexts. Groups with operators allowed an easy notation of the group operation. Instead of working with different symbols to denote different representations of the same group, one could simply use the group element to operate on the representation space. Thus the notation becomes somewhat simplified.

The concept of group with operators allowed an easy and short introduction to representation theory from the point of view of modern algebra. This kind of approach was quite original. However, as far as I know, it was not followed up by anyone else. Van der Waerden used it in later editions of the book, even though the concept had come out of fashion. Van der Waerden's approach was not fully modern, since he did not develop the theory in its full generality, but only in so far as it was necessary to introduce representation theory of groups. Thus, he tailored his modern approach to the needs of physicists.

## Slater's Method Revisited

In the letter to van der Waerden mentioned earlier, Ehrenfest characterized the appearance of group theory in quantum mechanics as “group plague” (*Gruppenpest*). As already mentioned he did not intend to get rid of it altogether—as one would with a real outbreak of the plague, but he tried to master this new set of mathematical tools. The resistance to group theory grew when the young American physicist J. C. Slater

---

<sup>33</sup>van der Waerden [1932, §11].

<sup>34</sup>Wigner [1931, p. 95].

<sup>35</sup>On the history of the representation theory of Lie groups see Hawkins [2000].

<sup>36</sup>Weyl [1931, chap. III, §6].

<sup>37</sup>Weyl [1931, p. VI.f.].



introduced a method in 1929 to determine the multiplet system of an atom with several electrons without using group theory.<sup>38</sup> Slater's method was warmly welcomed by the physicists' community. Many physicists believed that this was the beginning of the end of group theory in quantum mechanics. Slater remembered this as follows:

As soon as this paper [Slater, 1929] became known, it was obvious that a great many other physicists were disgusted as I [Slater] had been with the group-theoretical approach to the problem. As I heard later, there were remarks made such as "Slater has slain the 'Gruppenpest.'" I believe that no other piece of work I had done was so universally popular. [Slater, 1975, p. 62]

Slater's method rested on an approach developed by Hund who later became a colleague of van der Waerden in Leipzig.<sup>39</sup>

Van der Waerden introduced two methods to determine the multiplet structure of an atom with several electrons in his text book. He gave a very concise summary of the group-theoretical procedure without going into details but referring the reader instead to Weyl's text book. Van der Waerden then turned to Slater's alternative method. He introduced it in a positive light:

However, there is a second method, in principle already older, recently applied successfully in particular by J.C. SLATER, which gets by with much simpler aids and which does not require the representation theory of the permutation group.<sup>40</sup> [van der Waerden, 1932, p. 120, emphasis in the original]

Van der Waerden went on to explain Slater's method.<sup>41</sup> Group-theoretically speaking, Slater could avoid the permutation group by transforming the spin and the "place" of the electrons simultaneously and by taking only those configurations into account which give rise to antisymmetric wave functions. In a group-theoretic approach the permutation group could operate on both spaces separately. Then van der Waerden described Slater's method, which was based on a table of configurations, then converted into a graphical diagram and graphically analyzed. Instead of just copying this method, van der Waerden optimized it. His main achievement was to do away with the graphical part and to develop a purely computational algorithm instead. Firstly, van der Waerden shortened the table of configurations so that it only contained configurations that gave rise to an antisymmetric wave function and so that all configurations with negative values of  $M_S = \sum m_s$  were left out due to reasons of symmetry.

The following table (Table 1) shows van der Waerden's table of configuration for three electrons with  $n = 2$  and  $l = 1$ , i.e. three  $2p$  electrons.<sup>42</sup> The content of the round brackets symbolizes an electron with quantum numbers  $n, l, m_l$  and spin  $\pm 1/2$ . The left-hand side of each row is an abbreviation for an antisymmetric wave function which is

---

<sup>38</sup>Slater [1929].

<sup>39</sup>Hund [1927].

<sup>40</sup>"Es gibt aber eine zweite, im Prinzip schon ältere, neuerdings vor allem von J.C. SLATER erfolgreich angewendete Methode, die mit viel einfacheren Hilfsmitteln auskommt und insbesondere die Darstellungstheorie der Permutationsgruppe nicht benötigt."

<sup>41</sup>van der Waerden [1932, p. 120-124].

<sup>42</sup>van der Waerden [1932, p. 121].

**B. L. van der Waerden's Early Contributions to Quantum Mechanics**

---

			$M_L$	$M_S$
(2 1 1 +)	(2 1 0 +)	(2 1 -1 +)	0	3/2
(2 1 1 +)	(2 1 0 +)	(2 1 1 -)	2	1/2
(2 1 1 +)	(2 1 0 +)	(2 1 0 -)	1	-1/2
(2 1 1 +)	(2 1 0 +)	(2 1 -1 -)	0	-3/2
(2 1 1 +)	(2 1 -1 +)	(2 1 1 -)	1	-1/2
(2 1 1 +)	(2 1 -1 +)	(2 1 0 -)	0	-3/2
(2 1 1 +)	(2 1 -1 +)	(2 1 -1 -)	-1	-5/2
(2 1 0 +)	(2 1 -1 +)	(2 1 1 -)	0	-1/2
(2 1 0 +)	(2 1 -1 +)	(2 1 0 -)	-1	-3/2
(2 1 0 +)	(2 1 -1 +)	(2 1 -1 -)	-2	-5/2

Table 17.1: Van der Waerden's table of configurations for three  $2p$ -electrons

given by the following expression (e.g. for the first row):

$$\sum_{P \in S_3} \delta_P P \psi(2\ 1\ 1\ |q_1) \psi(2\ 1\ 0\ |q_2) \psi(2\ 1\ -1\ |q_3) u_1 v_1 w_1$$

in which  $S_3$  is the permutation group of three elements,  $\delta_P$  is the sign of the permutation,  $q_f$  a system of space coordinates of the  $f$ -th electron ( $f = 1, 2, 3$ ) and  $u_i, v_j, w_k$  ( $i, j, k = 1, 2$ ) are vector components in spin space with a 1 in the index indicating spin  $+1/2$  and a 2 indicating spin  $-1/2$ . In the second column one adds up the  $m_l$  and in the third the spin of the electron configuration, giving rise to numbers  $M_L$  and  $M_S$ .

Secondly, van der Waerden gave a clear-cut procedure of how to find the pairs  $L, S$  of an arising multiplet directly from the table of configurations. The procedure was as follows: First, one has to choose the greatest value for  $M_S$  in the table (in this case  $3/2$ ). Together with the value  $M_L$  from the same row (in this case 0) it gives rise to a multiplet with  $L = M_L$  and  $S = M_S$ . In case of more rows with the same value  $M_S$ , you choose the row with the greatest value  $M_L$ . Then you delete from the table all rows with values  $M_S = S, S - 1, \dots, 0$  and  $M_L = L, L - 1, \dots, -L$  once. (In the example of  $S = 3/2, L = 0$ , one deletes two rows: 1st, 4th). Then you start the procedure again from the beginning. In the example this leads to the multiplets  $^4S, ^2D, ^2P$ .

Van der Waerden's third way of optimizing Slater's method was to give three rules. Some of these rules were already implicitly used by Slater in his examples. The first rule stated that one could neglect the electron of a full shell (same  $n, l$  for  $2(2l + 1)$  electrons). The second one described how to construct the multiplets of the whole system from multiplets arising from subsystems. As subsystems he considered electrons in the same shell, i.e. sets of equivalent electrons (same  $n, l$ ). The third rule made use of the symmetry of the multiplet structure within a shell to determine the multiplets. At the end of the passage, van der Waerden gave a list of the possible multiplets occurring in shells up to  $l = 2$ . This list could be used as a table of reference by the working physicist when determining the multiplet structure of an atom with several electrons.

So, van der Waerden took on board the concerns of those physicists who were interested in easy calculational techniques. He restricted the use of group theory to a minimum. When it was possible to use a mathematically simpler method he did not hesitate to do

so. This again is a very pragmatic attitude, which is not at all in line with the modern algebraic way of reasoning. The inclusion of Slater's method into his book might also indicate that it was a method used by the physicists in Leipzig—after all Slater's method was based on method developed by Hund.

Van der Waerden's approach to Slater's method also differed considerably from Weyl's and Wigner's. Both of them explained the group-theoretic approach and gave all the mathematical details. Weyl did not mention Slater's method explicitly in his second edition of 1931, but implicitly referred to it.<sup>43</sup> In his preface Weyl alluded also to Slater's method:

It has recently been said that the "group plague" will gradually be taken out of quantum physics. This is definitely not true with respect to the group of rotations and of Lorentz-transformations. As to the group of permutations, its study really seems to include a detour due to the Pauli principle. Nevertheless, the representations of the group of permutations must remain a natural tool of theory, as long as one takes the existence of spin into account, but neglects its dynamic effect and as long as one wants to have a general overview of the resulting circumstances.<sup>44</sup> [Weyl, 1931, p. viif]

Weyl acknowledged that the permutation group could be avoided—at least to a certain extent—because of the Pauli principle, a principle which was also at work in Slater's method. Yet, he also insisted that the representation theory of the permutation group could not be avoided generally. Van der Waerden presented Slater's method as a shortcut around the representation theory of the permutation group for determining the multiplet system.

What about Wigner? Like van der Waerden, he mentioned Slater's theory. However, Wigner explained why Slater's method worked from a group-theoretic point of view. He groupified Slater's method, so to speak. In this way, he could also determine its range of applicability. Slater's method was restricted to particles of spin one half. The group-theoretic method, however, worked for particles with arbitrary spin. So, Wigner pointed to a physical reason which spoke in favour of the more complicated group-theoretic method.

---

<sup>43</sup>Slater's article was mentioned in two footnotes but only because of Slater's innovative approach in perturbation theory to calculate energy levels [Weyl, 1931, p. 173, fn. 4; p. 314, fn. 15].

<sup>44</sup>"Es geht in jüngster Zeit die Rede, daß die „Gruppenpest“ allmählich wieder aus der Quantenphysik ausgeschieden wird. Dies ist gewiss unrichtig, bezüglich der Rotations- und Lorentz-Gruppe. Was die Permutationsgruppe anlangt, so scheint ihr Studium in der Tat wegen des Pauliverbots einen Umweg einzuschließen. Dennoch müssen die Darstellungen der Permutationsgruppe ein natürliches Werkzeug der Theorie bleiben, solange die Existenz des spins berücksichtigt, seine dynamische Einwirkung aber vernachlässigt wird und man die daraus resultierenden Verhältnisse allgemein überblicken will." The given translation is closer to the German original than that of the English edition of 1950. The appreciative mentioning of Slater's works together with those of D. R. Hartree and Dirac by Weyl at the end of the paragraph (from which the above quote was taken) is done in the context of *numerical* methods in perturbation theory and thus, in my opinion, does not refer to Slater's method to avoid group-theoretic reasoning (see also previous footnote).

## Conclusion

The examples chosen to illustrate van der Waerden's approach failed to give a really coherent picture. The first example of the spinor calculus shows that van der Waerden developed a calculus at the request of Ehrenfest, that he tried to use as little mathematics as possible. No modern algebra went into this work. Instead a calculus was modelled on the tensor calculus. The second example—groups with operators—shows that he confronted the physicists with a new concept of modern algebra. However, the purpose of the concept was only to give an introduction to representation theory. Moreover, van der Waerden used the concept in a very limited way, adapted to the representation theory of groups. The third example shows that van der Waerden was a pragmatic person who included and improved Slater's method for reasons of simplicity. This is quite remarkable for a book dealing with group-theoretic methods.

What can we conclude from this? Van der Waerden did not aim to apply modern algebraic methods to quantum mechanics. It was not his main interest to demonstrate the power of group theory. I think he really intended to help those physicists like Ehrenfest to understand these new methods and to be able to work with them. Of course, by doing so he helped to spread and advance the new method.

However, I think, this was not intended as “fighting back” as J. Mehra and H. Rechenberg put it pointedly.<sup>45</sup> In my opinion, it was intended as a contribution to assist physicists—not in an arrogant way, but rather in a friendly, helpful way. This is indicated by the influence of “local” physicists on van der Waerden's research.<sup>46</sup>

## References

- Chayut, M. (2001). From the periphery: the genesis of Eugene P. Wigner's application of group theory to quantum mechanics. *Foundations of Chemistry*, 3: 55–78.
- Corry, L. (1996). *Modern Algebra and the Rise of Mathematical Structures*, volume 17 of *Science Network, Historical Studies*. Birkhäuser, Basel, Boston, Berlin.
- Courant, R. and Hilbert, D. (1924). *Methoden der mathematischen Physik*, volume 1. Springer-Verlag, Berlin, 1st edition.
- Dirac, P. A. M. (1936). Relativistic wave equations. *Proceedings of the Royal Society of London*, 155: 447–459.
- Dold-Samplonius, Y. (1994). Bartel Leendert van der Waerden befragt von Yvonne Dold-Samplonius. *Internationale Zeitschrift für Geschichte und Ethik der Naturwissenschaften, Technik und Medizin*, 2(3): 129–147. Engl. transl.: Interview with Bartel Leendert van der Waerden, *Notices Am. Math. Soc.* 44, No. 3, 313–320, 1997.
- Dold-Samplonius, Y. (1997). In memoriam: Bartel Leendert van der Waerden. *Historia Mathematica*, 24(2): 125–130.

---

<sup>45</sup>Mehra and Rechenberg [chap. III.4(e) 200].

<sup>46</sup>Another example of this influence is the chapter on molecular spectra in [van der Waerden, 1932] which apparently was influenced by discussions with Hund [Kleint and Wiemers, 1993, p. 205, fn. 26].

- Ehrenfest, P. (1932). Einige die Quantenmechanik betreffende Erkundigungsfragen. *Zeitschrift für Physik*, 78: 555–559.
- Eisenreich, G. (1981). B. L. van der Waerdens Wirken von 1931 bis 1945 in Leipzig. In Beckert, H. and Schumann, H., editors, *100 Jahre Mathematisches Seminar der Karl-Marx-Universität, Leipzig*, pages 218–244. VEB Deutscher Verlag der Wissenschaften, Berlin.
- Frei, G. (1993). Dedication: Bartel Leendert van der Waerden. Zum 90. Geburtstag. *Historia Mathematica*, 20(1): 5–11.
- Frei, G. (1998). Zum Gedenken an Bartel Leendert van der Waerden (2.2.1903–12.1.1996). *Elemente der Mathematik*, 53(4): 133–138.
- Frei, G., Top, J., and Walling, L. (1994). A short biography of B. L. van der Waerden. *Nieuw Archief voor Wiskunde*, IV/12(3): 137–144.
- Goenner, H. (2004). On the history of unified field theory. *Living Reviews in Relativity*, 7(2): 1–151. Online Article: cited June 2nd, 2004, [WWW.LIVINGREVIEWS.ORG/LRR-2004-2](http://WWW.LIVINGREVIEWS.ORG/LRR-2004-2).
- Gross, H. (1973). Herr Professor B. L. van der Waerden feierte seinen siebzigsten Geburtstag. *Elemente der Mathematik*, 28: 25–32.
- Hawkins, T. (2000). *Emergence of the theory of Lie groups. An essay in the history of mathematics 1869–1926*. Sources and Studies in the History of Mathematics and Mathematical Physics. Springer, New York, Berlin, Heidelberg.
- Hund, F. (1927). Symmetriecharaktere von Termen bei Systemen mit gleichen Partikeln in der Quantenmechanik. *Zeitschrift für Physik*, 43: 788–804.
- Infeld, L. and van der Waerden, B. L. (1933). Die Wellengleichung des Elektrons in der allgemeinen Relativitätstheorie. *Sitzungsberichte der Preussischen Akademie der Wissenschaften*, 7/10: 380–401. Corrections in: 11/13: 474.
- Jahn, H. A. (1935). Rotation und Schwingung des Methanmoleküls. *Annalen der Physik*, 23: 529–554.
- Kleint, C. and Wiemers, G., editors (1993). *Werner Heisenberg in Leipzig 1927–1942*. Akademie Verlag, Berlin. Abhandlung der Sächsischen Akademie der Wissenschaften zu Leipzig, Mathematisch-naturwissenschaftliche Klasse, Band 58, Heft 2.
- Krull, W. (1925). Über verallgemeinerte endliche Abelsche Gruppen. *Mathematische Zeitschrift*, 23: 161–196.
- Krull, W. (1926). Theorie und Anwendung der verallgemeinerten Abelschen Gruppen. *Sitzungsberichte der Heidelberger Akademie der Wissenschaften*, (1): 1–32.
- Laporte, O. and Uhlenbeck, G. E. (1931). Application of spinor analysis to the Maxwell and Dirac equations. *Physical Review*, 37: 1380–1397.

## B. L. van der Waerden's Early Contributions to Quantum Mechanics

---

- Mackey, G. W. (1988a). Hermann Weyl and the application of group theory to quantum mechanics. In Deppert, W., Hübner, K., Oberschelp, A., and Weidemann, V., editors, *Exact Sciences and their Philosophical Foundations. Vorträge des Internationalen Hermann-Weyl-Kongresses, Kiel 1985*, pp. 131–159. Peter Lang, Frankfurt am Main, Bern, New York, Paris.
- Mackey, G. W. (1988b). Weyl's program and modern physics. In Bleuler, K. and Werner, M., editors, *Differential geometrical methods in theoretical physics (Como, 1987)*, pp. 11–36. Kluwer, Dordrecht.
- Mehra, J. and Rechenberg, H. (2000). *The historical development of quantum theory: the completion of quantum mechanics 1926–1941: the probability interpretation and the statistical transformation theory, the physical interpretation and the empirical and mathematical foundations of quantum mechanics 1926–1932*, volume 6. Springer, New York, Heidelberg, Berlin.
- Noether, E. (1927). Abstrakter Aufbau der Idealtheorie in algebraischen Zahl- und Funktionenkörpern. *Mathematische Annalen*, 96: 26–61.
- Noether, E. (1929). Hyperkomplexe Größen und Darstellungstheorie. *Mathematische Zeitschrift*, 30(5): 641–692.
- Schappacher, N. (2003). A historical sketch of B. L. van der Waerden's work on algebraic geometry 1926–1946. In Gray, J. and Parshall, K. H., editors, *Proceedings of 2003 MSRI Conference on the History of Algebra*, pages 1–36. (To appear) Online manuscript: cited August 3, 2006: [WWW-IRMA.U-STRASBG.FR/SCHAPPA/VDWMSRI4.PDF](http://WWW-IRMA.U-STRASBG.FR/SCHAPPA/VDWMSRI4.PDF).
- Schlote, K.-H. (2007). *Zu den Wechselbeziehungen zwischen Mathematik und Physik an der Universität Leipzig in der Zeit von 1905 bis 1945*. Harri Deutsch, Frankfurt am Main. To appear.
- Schmidt, O. (1928). Über unendliche Gruppen mit endlicher Kette. *Mathematische Zeitschrift*, 29: 34–41.
- Scholz, E. (2006). Introducing groups into quantum theory (1926–1930). *Historia Mathematica*, 33: 440–490.
- Scriba, C. J. (1996a). Bartel Leendert van der Waerden 1903–1996. *Die Mitteilungen der Mathematischen Gesellschaft in Hamburg*, 15: 13–18.
- Scriba, C. J. (1996b). Bartel Leendert van der Waerden 2. Februar 1903 – 12. Januar 1996. *Berichte zur Wissenschaftsgeschichte*, 19: 245–251.
- Sigurdsson, S. (1991). *Hermann Weyl, Mathematics and Physics, 1900–1930*. PhD thesis, Harvard University.
- Slater, J. C. (1929). The theory of complex spectra. *Physical Review*, 34(10): 1293–1322.

- Slater, J. C. (1975). *Solid State and Molecular Theory. A Scientific Biography*. J. Wiley, New York.
- Soifer, A. (2004a). In search of van der Waerden: Leipzig and Amsterdam, 1931–1951: Part I: Leipzig. *Geombinatorics*, 14(1): 21–40.
- Soifer, A. (2004b). In search of van der Waerden: Leipzig and Amsterdam, 1931–1951: Part II: Amsterdam, 1945. *Geombinatorics*, 14(2): 72–102.
- Soifer, A. (2005). In search of van der Waerden: Leipzig and Amsterdam, 1931–1951: Part III: Amsterdam, 1946–1951. *Geombinatorics*, 14(3): 124–161.
- Thiele, R. (2004). Van der Waerdens Leipziger Jahre 1931–1945. *Mitteilungen der Deutschen Mathematiker-Vereinigung*, 12(1): 8–20.
- Top, J. and Walling, L. (1994). Bibliography of B. L. van der Waerden. *Nieuw Archief voor Wiskunde*, 12(3): 179–193.
- van der Waerden, B. L. (1921). Over Einsteins relativiteitstheorie. *De socialistische gids*, 6: 54–73, 185–204.
- van der Waerden, B. L. (1929). Spinoranalyse. *Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen, Mathematisch-Physikalische Klasse*, ohne Angabe: 100–109.
- van der Waerden, B. L. (1930). *Moderne Algebra*, volume 1. Julius Springer, Berlin, 1st edition.
- van der Waerden, B. L. (1931). *Moderne Algebra*, volume 2. Julius Springer, Berlin, 1st edition.
- van der Waerden, B. L. (1932). *Die gruppentheoretische Methode in der Quantenmechanik*. Julius Springer, Berlin. (reprinted by Edward Brothers, Ann Arbor, 1944; 2nd (Engl.) revised edition: *Group theory and quantum mechanics*, 1974).
- van der Waerden, B. L. (1941). Die lange Reichweite der regelmäßigen Atomanordnung in Mischkristallen. *Zeitschrift für Physik*, 118: 473–488.
- van der Waerden, B. L. (1960). Exclusion principle and spin. In Fierz, M. and Weiskopf, V. F., editors, *Theoretical physics in the twentieth century. A memorial volume to Wolfgang Pauli*, pp. 199–244. Interscience Publishers Inc., New York, London.
- van der Waerden, B. L. (1963). Zur Quantentheorie der Wellenfelder. *Helvetica Physica Acta*, 36: 945–962.
- van der Waerden, B. L. (1966). On measurements in quantum mechanics. *Zeitschrift für Physik*, 190: 99–109.
- van der Waerden, B. L., editor (1967). *Sources of quantum mechanics*. North-Holland Publishing Company, Amsterdam.

## B. L. van der Waerden's Early Contributions to Quantum Mechanics

---

- van der Waerden, B. L. (1973). From matrix mechanics and wave mechanics to unified quantum mechanics. In Mehra, J., editor, *The physicist's conception of nature*, pages 276–293. Reidel, Dordrecht.
- van der Waerden, B. L. (1975). *Mathematik für Naturwissenschaftler*. Bibliographisches Institut, Mannheim, Wien, Zürich.
- van der Waerden, B. L. (1976). Gedenkrede Werner Heisenberg. *Berichte und Mitteilungen der Max Planck-Gesellschaft*, pp. 17–22. Sonderheft.
- van der Waerden, B. L. (1983). The school of Hilbert and Emmy Noether. *The Bulletin of the London Mathematical Society*, pp. 1–7.
- van Dongen, J. (2004). Einstein's methodology, semivectors and the unification of electrons and protons. *Archive for History of Exact Sciences*, 58: 219–254.
- Weiß, E. A. (1924). *Ein räumliches Analogon zum Hesseschen Übertragungsprinzip*. PhD thesis, Rheinische Friedrich-Wilhelms-Universität Bonn, Greifswald.
- Weyl, H. (1925). Theorie der Darstellung kontinuierlicher halbeinfacher Gruppen durch lineare Transformationen I. *Mathematische Zeitschrift*, 23: 271–301.
- Weyl, H. (1926). Theorie der Darstellung kontinuierlicher halbeinfacher Gruppen durch lineare Transformationen II. *Mathematische Zeitschrift*, 24: 328–376.
- Weyl, H. (1928). *Gruppentheorie und Quantenmechanik*. Hirzel, Leipzig.
- Weyl, H. (1929). Elektron und Gravitation I. *Zeitschrift für Physik*, 56: 330–352.
- Weyl, H. (1931). *Gruppentheorie und Quantenmechanik*. Hirzel, Leipzig, 2nd revised edition. Engl. transl. by H. P. Robertson: *The theory of groups and quantum mechanics*, New York 1950.
- Wigner, E. (1931). *Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspektren*. Vieweg, Braunschweig. (Reprinted by Edwards Brothers, Ann Arbor, 1944; Engl. transl. by James J. Griffiths: *Group theory and its application to the quantum mechanics of atomic spectra*, New York, 1959).





# 18 Engineering Entanglement: Quantum Computation, Quantum Communication, and Re-conceptualizing Information

CHEN-PANG YEANG

## Introduction: the EPR Paradox and Entanglement

Very few issues in the history of quantum mechanics have undergone so many twists as entanglement. According to the received view, the idea of entanglement was proposed as a paradox to challenge quantum mechanics. Albert Einstein, the major opponent of the Copenhagen interpretation, disagreed with Werner Heisenberg and Niels Bohr's denial of physical reality without the intervention of measurement, which they claimed to be an implication of quantum mechanics. From the late 1920s to the early 1930s, Einstein exchanged a series of arguments with Bohr regarding the consistency of the Copenhagen interpretation. The pinnacle of this debate was a thought experiment that Einstein, his assistant Nathan Rosen at the Institute for Advanced Study, and the Russia-born physicist Boris Podolsky came up in 1935.

What is now famous as the Einstein-Podolsky-Rosen (EPR) experiment works as follows: Generate two identical particles at some location and let them move away. According to quantum mechanics, these two particles together constitute a single quantum state that can be expressed by a wave function. Prepare the two particles at a particular quantum state<sup>1</sup> (the "EPR" or "entangled" state) so that they correlate perfectly with each other. For the EPR state, it can be shown that when one makes a momentum measurement at particle 1 and obtains the result  $p$ , she can be sure that were she to measure the momentum of particle 2 she would get  $-p$ . Similarly, when she measures the position of particle 1 and obtains  $x$ , she is guaranteed to get  $-x-x_0$  from measuring the position of particle 2 ( $x_0$  is a constant). In brief, when the two-particle system is at the EPR state, measuring the momentum or position of one particle is sufficient to determine the other particle's momentum or position.

This seemingly straightforward scenario was nonetheless turned into EPR's weapon against the completeness of quantum mechanics. From Heisenberg's interpretation of the uncertainty principle, one cannot determine simultaneously the momentum and position (or any other non-commuting conjugate pair) of a particle, because one measurement would perturb the particle's original state and thus affect the accuracy of the other

---

<sup>1</sup>The wave function is  $\Psi(x_1, x_2) = \int_{-\infty}^{\infty} e^{i2\pi/h(x_1 - x_2 + x_0)p} dp$ . See Albert Einstein, Boris Podolsky, and Nathan Rosen, "Can quantum-mechanical description of physical reality be considered complete?" *Physical Review*, 47 (1935), 779, equation (10).

measurement. In the above thought experiment, however, one can determine particle 2's momentum or position without any measurement-induced perturbation, since all the measurements are done at particle 1. To EPR, that means both momentum and position are pre-existing physical properties (in EPR's words, "elements of physical reality") of particle 2. Constrained by the uncertainty principle, quantum mechanics cannot yield accurate predictions of the second particle's momentum and position at the same time. But it does not imply (contra Bohr and Heisenberg) that nature prohibits simultaneous determination of both physical quantities. Rather, it indicates that quantum mechanics fails to capture all the elements of physical reality. Quantum mechanics is incomplete.<sup>2</sup>

The entangled state epitomized physicists' efforts to understand the strange, counter-intuitive characteristics of quantum mechanics. Since the founding of the "new" quantum mechanics in the mid-1920s, physicists have tried to grapple with various consequences of the theory that appeared contradictory to the established worldview: An object does not proceed along a trajectory but has the probability to be everywhere. Particles "interfere" with one another to form wavelike patterns. Entities far apart have non-local, spontaneous correlations. Measurement determines physical reality. Entanglement was not the only scenario for illustrating and exploring these odd features of quantum mechanics. Nor did it start as a very conspicuous one. (The EPR paper did not incur much response in the first two decades after its publication.) With a few physicists' rediscovery and elaboration in the 1950s–60s, however, entanglement became one of the most important avenues for the study of quantum logic and the axiomatic foundation of quantum physics.

For instance, the maverick American physicist David Bohm used entanglement in developing his non-local hidden-variable interpretation of quantum mechanics. In 1957, Bohm and his collaborator Yakir Aharonov of Haifa, Israel, reformulated the EPR scenario from its original momentum-position basis into a simpler basis involving spins<sup>3</sup>. In Bohm and Aharonov's version, each of the two particles was described by two quantum states—spin up ( $|0\rangle$ ) and spin down ( $|1\rangle$ )—instead of the continuous states representing momentum and position. Then the wave function of the EPR state was

$$|\text{EPR}\rangle = \frac{1}{\sqrt{2}}(|0\rangle|1\rangle - |1\rangle|0\rangle) \quad (18.1)$$

This reformulation of the EPR state turned out to be essential. In his visit to the United States in 1964, the Irish particle physicist John Stewart Bell of CERN discovered a way to respond to EPR's paradox based on the Bohmian entangled state. Bell found that if quantum mechanics were incomplete (as EPR held) and the two particles of the Bohmian entangled state were determined by two sets of unknown parameters independent of each other (i.e., two sets of local hidden variables), then the probabilities of the events for the two particles would follow the so-called "Bell inequalities." However, the probabilities of such events obtained from quantum mechanical calculations did not obey the Bell inequalities. Therefore, any local hidden-variable theory of quantum mechanics must be contradictory.<sup>4</sup>

---

<sup>2</sup>*Ibid*, 777–780.

<sup>3</sup>David Bohm and Yakir Aharonov, "Discussion of experimental proof for the paradox of Einstein, Rosen, and Podolsky," *Physical Review*, 108 : 4 (1957), 1070–1076.

<sup>4</sup>John S. Bell, "On the Einstein-Podolsky-Rosen paradox," *Physics* 1 (1964), 195–200; reprinted in

From Einstein, Podolsky, Rosen, to Bohm, Aharonov, Bell, and their followers in the 1960s–70s, those working on entanglement were preoccupied with understanding the conceptual foundation of quantum mechanics. They treated the entangled state as a model scenario to demonstrate how weird the quantum world is and to interpret why it is the case. To the physicist community, the EPR problem was associated with the meta-theoretical issues of quantum mechanics, such as realism, quantum logic, axiomatic formulation, hidden-variable interpretations, completeness, and measurements.

Nevertheless, an epistemic change has emerged in the past thirty years. Since the 1980s, a number of scholars have revived the study of entanglement for a quite different reason. In addition to the meta-theoretical concerns with the foundation of quantum mechanics, they broadened their attention to the pragmatic aspects of entanglement. Some of them even set aside the question of *why* quantum mechanics is so strange and rather focused on *how to utilize* the strange properties of quantum mechanics. Their answer gave rise to a new field known as quantum information.

How did such an epistemic shift occur? This paper examines the rise and ongoing development of quantum information, the applications of quantum principles to computation, communications, and other information processing problems. Although entanglement is not the only substantial element of quantum information, it nonetheless constitutes the intellectual core of quantum information and has played a key part in the history of this new field. Specifically, entanglement has been transformed from an *explanandum* in the meta-theoretical inquiries of quantum mechanics into a *resource* that facilitates tasks such as parallel computing, teleportation, super-dense coding, and cryptography. In this paper, I will argue that the development of quantum information can be viewed as a process in which scientists and technologists learned how to *engineering* entanglement and related behaviors of single quantum states.

It is worth noting that “engineering” in the history of quantum information has several unconventional senses, all of which are significant in different ways. First, unlike most applied outgrowths of quantum mechanics—microelectronics, chemistry, material science—that deal with macroscopic physical systems with many atoms or molecules, quantum information treats single atoms and coherent quantum states. Thus, the relevant engineering is not doping materials with impurities or changing their statistical mechanical conditions. Rather, it consists of preparing single atoms at simple quantum states, carefully changing these states, and following their amplitude and phase variations. The manipulation of single, coherent quantum states has become an indispensable aspect of engineering. Second, the part theory plays in engineering is no longer restricted to modeling and analysis of some given working systems. In quantum information (as well as in computer and communications sciences), theory is also used to gauge the performance of *all possible* working systems and thus to predict the *fundamental limit* of all solutions to an engineering problem. In other words, engineering consists of figuring out not only what can be done, but also what cannot be done. Third, a major challenge in quantum information is to find how to utilize quantum characteristics such as entanglement. As we will see, a quantum computer or quantum channel does not offer easy access to the information it carries, and often it is not more effective than its classical counterpart. Therefore, some “killer applications” are critical. In fact, the field began

---

John S. Bell, *It Speakable and Unspeakable in Quantum Mechanics: Collected Papers on Quantum Philosophy* (Cambridge: Cambridge University Press, 2004), 14–21.

to take off only after some specific algorithms, such as quantum factorization and quantum search, were developed in the early 1990s. To this date, we may still characterize quantum information as “an approach looking for problems.” In this sense, engineering also included the identification of proper problems.

From the above discussion, it should be clear that the history of quantum information involved multiple intellectual traditions of different communities. The most obvious tradition was the one shared by the physicists working on the EPR paradox and related meta-theoretical issues in quantum mechanics. Yet these physicists/philosophers were by no means the only historical actors in the development of quantum information. There were also down-to-the-earth contributors who cared more about the nitty-gritty details of calculations and experiments than about the philosophical implications: mathematicians and computer scientists preoccupied with universal computing, algorithms, and complexity, information theorists trying to approach the channel capacity with better communications codes, experimental atomic physicists working on purifying and manipulating single atoms, and optoelectronic engineers designing laser circuits. These peoples entered the history of quantum information at different stages.

### Conceiving Quantum Computers

The origin of the idea of quantum computers was closely related to the discussions on universal computation in the first half of the twentieth century. In 1936, the American logician Alonzo Church and the English mathematician Alan Turing independently proposed a solution to David Hilbert’s *Entscheidungsproblem*. Their proposal ended up with what is now known as the “Church-Turing thesis:” every “computable” function (i.e., function that can be computed by an algorithm) can be computed by a certain generic procedure. In Turing’s version, such a generic procedure was a “universal Turing machine.” The Turing machine was a general computing architecture, not a real computer. It comprised a program, a finite-state control, an infinite one-dimensional tape, and a read/write head (see Figure 1). When the machine executed a computing task, the program instructed the finite-state control to move the read/write head according to the machine’s internal state and the data being accessed on the tape’s cell. The read/write head could read the data on the cell, overwrite the data, or simply skip to the next cell. The Church-Turing thesis asserted that this primitive architecture could perform all the tasks any digital computer could carry out (see Fig. 18.1).<sup>5</sup>

The Church-Turing thesis and the universal Turing machine laid out the foundation for modern computer science. However, they also left a longstanding puzzle: Like all the digital computers, the Turing machine performs a discrete sequence of operations that are irreversible—a simple way to understand why it is the case is to observe that all these computing operations can be represented by logic circuits containing AND, OR, and NOT gates; but the AND and OR gates are not reversible operators since they take two inputs but give only one output. Nevertheless, many physical processes in nature (including those in classical and quantum mechanics) are reversible. Thus, why and how is it possible to implement a universal computer with a physical means? An obvious

---

<sup>5</sup> Alan Turing, “On computable numbers, with an application to the Entscheidungsproblem,” *Proceedings of the London Mathematical Society*, [series 2] 42 (1936–37), 230–265; Michael A. Nielsen and Isaac L. Chuang, *Quantum Computation and Quantum Information* (Cambridge: Cambridge University Press, 2000), 122–125.

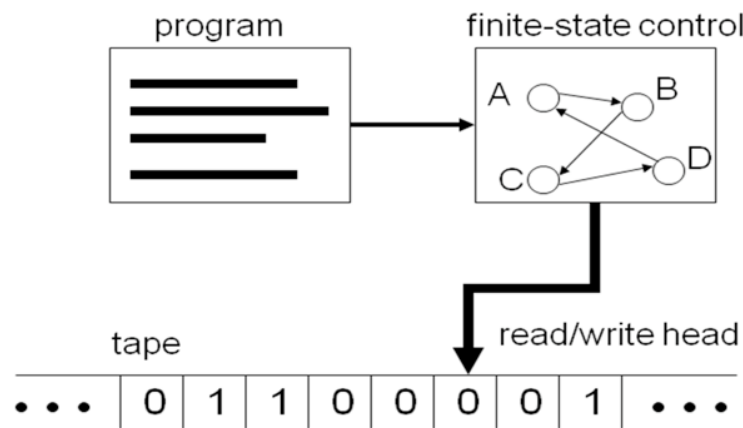


Figure 18.1: Universal Turing Machine

answer is thermodynamics and statistical mechanics, since they describe irreversible physical processes. Yet, the universal Turing machine as an irreversible process has its disorderliness (or entropy) decrease with time, which is apparently inconsistent with the second law of thermodynamics. So the problem remains unsolved.

In the 1960s–80s, the close study of this problem led to the expansion of a new area, physics of computation. Rolf Landauer and Charles Bennett at IBM Thomas Watson Research Center, Tommaso Toffoli at MIT Laboratory of Computer Science, and Edward Fredkin at Boston University were the leading figures in this area. It would be beyond the scope of this paper to delve into its immense literature. Suffice to point out that the problem of implementing the irreversible universal computer with a physical process yielded two related problems: Is it possible to make a *reversible* universal computer? Can we simulate every physical process with a universal computer? To deal with the first problem, Bennett, Fredkin, and Toffoli respectively introduced reversible Turing machines and reversible logic circuits.<sup>6</sup> The grappling of the second problem made room for the notion of quantum computers.

The idea of quantum computing began to appear in the 1970s. But perhaps the first influential literatures on this subject were introduced at the conference “Physics and Computation” that Fredkin, Landauer, and Toffoli co-organized at MIT in May 1981. At the conference, both Paul A. Benioff of the Argonne National Laboratory and Richard Feynman, then professor at Caltech, presented this idea. Benioff’s was a model of classical Turing-like computation that could be implemented with quantum kinematics and dynamics<sup>7</sup>. Feynman’s was something different. He started his presentation by remarking that he wanted to talk about the problem of “simulating physics with computers.”<sup>8</sup>

<sup>6</sup>Charles H. Bennett, “Logical reversibility of computation,” *IBM Journal of Research and Development*, 17 : 6 (1973), 525–532; Edward Fredkin and Tommaso Toffoli, “Conservative logic,” *International Journal of Theoretical Physics*, 21 : 3/4 (1982), 219–253.

<sup>7</sup>Paul A. Benioff, “Quantum mechanical Hamiltonian models of discrete processes that erase their own histories: application to Turing machines,” *International Journal of Theoretical Physics*, 21 : 3/4 (1982), 177–201.

<sup>8</sup>Richard Feynman, “Simulating physics with computers,” *International Journal of Theoretical Physics*,

Classical physics, according to Feynman, may be efficiently simulated by conventional digital computers such as the Turing machines, since the relevant physical problems can be described as differential equations and solved numerically by algorithms. And this approach applies to a stochastic physical system as long as some randomized features are introduced into the Turing machines. But the same approach would encounter difficulties in simulating quantum physics, for the quantum wave functions do not represent ordinary probabilities. Instead, they exhibit a variety of strange features pertinent only to quantum mechanics (such as interference, indeterminacy, non-locality, and the violation of the Bell inequalities). In fact, in order to simulate a quantum system, a classical computer needs an exponentially huge memory to cover the entire Hilbert space. (An  $N$ -level quantum system with  $R$  particles has  $N^R$  configurations in total.) Therefore, Feynman argued, a more efficient means to simulate quantum physics is the quantum computer. He went further to propose a universal quantum simulator comprising a lattice of spin-up or spin-down particles (like an Ising model) with nearest-neighbor interactions that could be freely specified, and speculated that this system could be used to simulate many quantum field problems.<sup>9</sup>

Feynman's quantum machine was more a simulator than a computer in Turing's sense. The individual pushing the idea of quantum computer further toward the Turing-like, algorithmic direction was David Deutsch. Born in Haifa, Israel, Deutsch received his undergraduate education at Cambridge and Oxford and spent some years as a physics graduate student at the University of Texas at Austin. Deutsch's original interest lay in cosmology. While in Austin, he studied quantum field theory in general relativistic space-time. The Austin years shaped his intellectual path. As he later recalled, the scientists that gave him most influence on his work were Dennis Sciama, John Wheeler, and Bryce de Witt, all taught in the Physics Department of UT Austin when Deutsch studied there. De Witt played an especially important part. In Deutsch's own words, "he was the one who introduced me to Everett's many-worlds interpretation of quantum mechanics, and to the wider implications of quantum field theory, and it was because of his take on both the formalism and interpretation of quantum mechanics that I got interested in quantum computers."<sup>10</sup>

Deutsch did not follow his mentors in Texas to pursue cosmology and astrophysics, though. He returned to England, obtained a position as a researcher in the Department of Astrophysics at Oxford University, and started working on quantum computing. In 1985, he published a seminal paper on the topic in *Proceedings of the Royal Society of London*. Entitled "Quantum theory, the Church-Turing principle, and the universal quantum computer," this paper began with a challenge to classical universal computers that was similar to Feynman's: The universal Turing machine can compute every computable function, but can it be used to simulate every finitely realizable physical system? Like Feynman, Deutsch gave a negative answer to the question, owing to various constraints of the classical computation model. To fulfill both the mathematical and the physical universality, Deutsch developed a quantum version of the universal Turing machine. This quantum universal Turing machine contained the same elements as

---

21 : 6/7 (1982), 467.

<sup>9</sup>*Ibid*, 474-476.

<sup>10</sup>Filiz Peach's interview with David Deutsch in *Philosophy Now*, 30 December 2000 (<http://www.qubit.org/people/david/Articles/PhilosophyNow.html>); "David Deutsch," in Edge: The Third Culture (<http://www.edge.org/3rd.culture/bios/deutsch.html>).

its classical counterpart—a program, a finite-state controller, a tape, and a read/write head. Contrasting the classical computer, however, the internal states of this quantum computer and its data recorded on the tape memory were both quantum states following the quantum principles such as Hilbert-space expansion, superposition, non-locality, etc. Moreover, all operations of the machine, including the transition from one internal state to another and the writing of a piece of quantum data on the tape, corresponded to unitary operators on quantum states and thus are reversible. Deutsch showed that this quantum Turing machine was able to compute every mathematical function that was computable by a classical Turing machine or a randomized classical Turing machine. Moreover, since the quantum Turing machine was reversible and operates on quantum mechanical principles, it could be used to simulate efficiently the classical and quantum physical systems. Feynman’s dream was fulfilled.<sup>11</sup>

The history of quantum computing would have been much more limited if Deutsch had stopped here. Although the universal quantum Turing machine could do anything that classical Turing machines could do, it was not clear at this moment whether this quantum computer could do anything that the classical computers could *not* do (except for simulating quantum physics) or perform any task more efficiently than the classical computers. Without the last two features, the quantum computers were at best equivalent to conventional computers, meaning it did not make sense to explore further the quantum computers from the practical point of view. Deutsch was aware of this problem and had a solution to it. He contended that the quantum computers were not only equivalent to classical computers; they were more efficient than the latter for some kinds of computing tasks (in addition to simulating quantum physics). The fundamental superiority of quantum computers, Deutsch argued, was based upon what he called “quantum parallelism,” a basic property of quantum mechanics. Deutsch demonstrated the idea of quantum parallelism with a simple example. In the quantum world, the state of a particle can be a superposition of all basis states. Prepare a particular, “mixed” quantum state in an  $N$ -state system:

$$|\psi\rangle = \frac{(|0\rangle + |1\rangle + \dots + |N - 1\rangle)}{\sqrt{N}} .$$

Couple this particle with another particle at state  $|0\rangle$ . The composite two-particle system has the quantum state

$$|\psi0\rangle = \frac{(|00\rangle + |10\rangle + \dots + |N - 1, 0\rangle)}{\sqrt{N}} .$$

Deutsch showed that there exists a quantum operation (or a quantum program) that leaves the first “slot” of each term unchanged while registers the result of evaluating a function  $f$  at the second “slot:” . Thus the composite state after the operation becomes

$$|\psi0\rangle \mapsto |\phi\rangle = \frac{(|0, f(0)\rangle + |1, f(1)\rangle + \dots + |N - 1, f(N - 1)\rangle)}{\sqrt{N}} .$$

This final state has a great computational advantage: It contains all the values of the function  $f$  at  $0, 1, \dots, N - 1$  in a single wave function, and this result is obtained only

---

<sup>11</sup>David Deutsch, “Quantum theory, the Church-Turing principle, and the universal quantum computer,” *Proceedings of the Royal Society of London A*, 400 : 1818 (1985), 97–107.



with a single quantum operation. The implication: parallel information processing is possible with a serial quantum computer.<sup>12</sup>

Quantum parallelism and entanglement are the manifestations of the same quantum characteristics: The states of multiple particles can be expressed as linear combinations of the basis states, and the composite resulting state is the sum of couplings between the terms in these linear combinations. Deutsch's identification of the potential applications of these characteristics marked a significant step toward quantum computation. Nevertheless, quantum parallelism was not easy to use as it appeared to be. Although Deutsch's simple example showed the promise of getting  $f(0), f(1), \dots, f(N - 1)$  at the output state  $|\phi\rangle$ , it was nonetheless difficult to retrieve all these values at the same time, since measuring  $|\phi\rangle$  with respect to any of the state  $|i, f(i)\rangle$  would inevitably collapse the original form of  $|\phi\rangle$  and destroy the information it contained about other  $f(\cdot)$ 's. This did not mean that quantum parallelism was doomed useless, but it did imply that more careful thoughts and more creative schemes were required to exploit quantum parallelism. Deutsch himself started developing one. Instead of retrieving all the  $f(\cdot)$ 's, he sought to obtain a global property of  $f(\cdot)$  (a property involving multiple evaluations of  $f$ ) from  $|\phi\rangle$ . With the even simpler binary case in which  $N = 2$  and  $f$  took only the value of 0 or 1, he demonstrated that the value  $f(0) \oplus f(1)$  ( $\oplus$  stands for the logical operation "Exclusive OR") could be determined by certain appropriate measurements of  $|\phi\rangle$ .<sup>13</sup>

## A Computer Looking for Algorithms

Deutsch became an advocate and devotee of quantum computation after the publication of his 1985 paper. In the second half of the 1980s, he moved to the Mathematical Institute of Oxford and worked on a general theory of quantum logical circuits to replace the less tractable quantum Turing machines. In computer science, a conventional digital computer was constituted of logical circuits with a few building blocks such as wires, sinks, and the AND, OR, and NOT gates. Deutsch's aim was to develop a theory for the necessary building blocks for all quantum logical circuits that shared the essential features of the classical logical circuits. The culmination of this work was a paper published in *Proceedings of the Royal Society of London* in 1989.<sup>14</sup> In this paper, Deutsch started to use the states  $|0\rangle$  and  $|1\rangle$  as the quantum counterparts of the classical bits 0 and 1. (In 1995, a quantum information theorist Benjamin Schumacher at Kenyon College of Ohio coined the term "qubits" to denote these quantum bits  $|0\rangle$  and  $|1\rangle$ .<sup>15</sup>) Deutsch also proposed a set of elementary building blocks for two-qubit quantum logical operations: the "swap gate" exchanging the order of the first and the second qubits, and the important "controlled-NOT gate" that left the first qubit intact while flipped the second qubit if the first qubit read 1. (This was an analogy of the "Toffoli gate," a reversible two-bit logical operation Toffoli had developed in the 1970s.) In the early 1990s, some one-qubit operations such as the Pauli spin matrices and the so-called "Hadamard matrix" were also added to the repertoire of the quantum logical gates.

---

<sup>12</sup> *Ibid*, 111–113.

<sup>13</sup> *Ibid*, 112

<sup>14</sup> David Deutsch, "Quantum computational networks," in *Proceedings of the Royal Society of London A*, 425:1868 (1989), 73–90.

<sup>15</sup> Benjamin Schumacher, "Quantum coding," *Physical Review A*, 51 : 4 (1995), 2747.

Despite the increasing knowledge on the foundation of quantum computation, the question of application remained: What is the quantum computer useful for? As Deutsch had observed, the idea of quantum computing might not be worth pursuing if there were no algorithm for this computer that was more efficient than the existing approaches to a certain computational task. In other words, a quantum computer must have impressive algorithms with practical potential. The developments of such algorithms in the 1990s marked the real take-off of quantum computation.

The first initiative was taken in Oxford. As early as 1985, Deutsch had come up with a quantum parallel algorithm that solved a simple problem: determining whether  $f(0) \oplus f(1)$  is 0 or 1. Although this did not address any “real” mathematical problem, it showed a vague but promising direction to go. To expand the algorithm in 1985, Deutsch sought the collaboration of another Oxford alumnus Richard Jozsa. Jozsa received his Ph.D. in physics at Oxford University under the supervision of the mathematical physicist Roger Penrose. Like Deutsch, Jozsa started as a cosmologist but ended up a specialist in the physics of computation. In 1992, the two colleagues published an algorithm, based on Deutsch’s 1985 scheme, to solve a less straightforward problem.<sup>16</sup>

The so-called “Deutsch-Jozsa algorithm” tackles the following problem: Consider a binary functions  $f$  that takes integer argument from 0 to  $2^n - 1$ . The function  $f$  is either *constant* (0 or 1) for all values of the argument, or *balanced* in the sense that  $f(x) = 0$  for half of the  $x$  between 0 to  $2^n - 1$  and 1 for the other half. The goal is to determine whether  $f$  is constant or balanced with the least number of operations. For the classical algorithms, the only general approach to this problem is to check the value of  $f(x)$  one by one, and it may take as many as  $2^{n-1} + 1$  checks before getting the answer. Nevertheless, Deutsch and Jozsa argued, an algorithm using the property of quantum parallelism can significantly reduce the number of operations. Key to the Deutsch-Jozsa approach is to prepare mixed  $(n+1)$  qubits exhausting all the quantum states from  $|0\rangle$  to  $|2^n - 1\rangle$  using the “Hadamard gates” (a Hadamard gate transforms  $|0\rangle$  into  $\frac{|0\rangle + |1\rangle}{\sqrt{2}}$  and  $|1\rangle$  into  $\frac{|0\rangle - |1\rangle}{\sqrt{2}}$ ). The overall output is then applied to the generalized controlled-NOT operation with  $n$  controlling qubits (representing a number  $x$ ) and 1 signal qubit (representing a number  $y$ ). While the first  $n$  qubits remain unchanged ( $x$ ), the signal qubit after the gate becomes  $y \oplus f(x)$ . Finally, the first  $n$  qubits ( $x$ ) are employed by the Hadamard gates again (see Figure 2 for the exact procedure). Deutsch and Jozsa showed that after all these operations, the first  $n$  qubits offer a straightforward test for the nature of  $f$ —it is constant if all the qubits are zero, and is balanced otherwise.

The strength of the Deutsch-Jozsa algorithm is its few number of operations compared to the conventional solutions to the same problem. While the conventional algorithms may take as many as  $2^n/2 + 1$  steps to determine the nature of  $f$ , the quantum algorithm takes a single step, for the information about all values of  $f$  is contained in the output quantum state. This is a significant saving of computational time, or, the reduction of computational complexity.

The Deutsch-Jozsa algorithm demonstrated the possibility of *engineering* the strange properties of quantum mechanics by turning them into computational resources. But

<sup>16</sup>David Deutsch and Richard Jozsa, “Rapid solutions of problems by quantum computation,” *Proceedings of the Royal Society of London A*, 439 : 1907 (1992), 553–558.

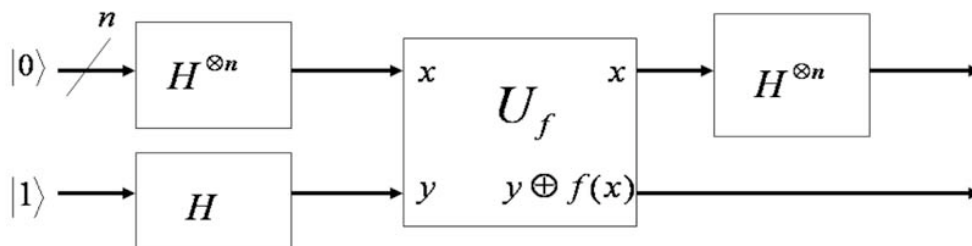


Figure 18.2: Deutsch-Jozsa Algorithm

the problem this algorithm aimed to solve was still artificial as well as insignificant, if not straightforward. Not until the mid-1990s did quantum computing begin to attack some “real-world” problems. Enter the American mathematician Peter Shor.

A native of California, Peter Shor was a mathematical prodigy—he won the International Olympiad and the Putnam Competition while in college. He received his B.S. from Caltech in mathematics and Ph.D. from MIT in applied mathematics. After graduation, he spent a year as a postdoc at the University of California in Berkeley and eventually landed a research position at the AT&T Bell Laboratories. Shor’s early mathematical interests focused on statistical and geometrical problems in computer science. His Ph.D. dissertation was about the probabilistic analysis of the “bin-packing” problem: to pack a number of objects with different volumes and shapes into the least number of fixed bins. From the 1980s to the early 1990s, he published in a variety of areas including discrete and computational geometry, applied probability, bin packing and scheduling, and combinatorics.<sup>17</sup> Compared with Deutsch and Jozsa, therefore, Shor received less training in quantum physics but was more sensitive to the ongoing development in computer science.

Shor’s involvement with quantum computers began in 1994, when he proposed a famous quantum algorithm capable of tackling several important problems in number theory. In a conference paper read at the *IEEE Annual Symposium on Foundations of Computer Science*, Shor claimed that he could use the property of quantum parallelism to solve the so-called “order-finding” problem with a quantum algorithm that had a significantly lower time complexity than the traditional approaches.<sup>18</sup> The order-finding problem can be stated as follows: Consider two positive integers  $x$  and  $N$ , where  $N > x$ . The order of  $x$  modulo  $N$  is defined as the smallest positive integer  $r$  so that  $x^r \equiv 1 \pmod{N}$  (note that  $A \equiv B \pmod{N}$  when  $A - B$  is a multiple of  $N$ ). The order-finding problem has been considered difficult. So far, no classical algorithms have been developed to solve the problem with the complexity (number of steps) lower than the polynomial orders of  $N$ . And most available algorithms do not go beyond trying different values of  $r$  one by one in the modulo equation. That is, there is not yet an “efficient” classical algorithm to perform order finding.<sup>19</sup>

Shor’s approach to this apparently intractable problem relied on Deutsch’s idea of

<sup>17</sup><http://www-math.mit.edu/~shor/pubs.html>.

<sup>18</sup>Peter W. Shor, “Algorithms for quantum computation: discrete logarithms and factoring,” *Proceedings of the 35th Annual Symposium on Foundations of Computer Science* (1994), 124–134.

<sup>19</sup>Nielsen and Chuang (2000), 226.

quantum parallelism, an entanglement-like resource to facilitate certain computations. First, Shor noticed that a Fourier transform could be employed on an arbitrary quantum state. Like Deutsch's parallel state that contained all the information about a function, this "quantum Fourier transform" condensed all the spectral data of the input state into the output superposition state. And since the quantum Fourier transform was a quantum operator, it could be implemented with the components of standard quantum circuits such as Hadamard gates and phase rotators. In Shor's circuit for the quantum Fourier transform for  $N$  elements, moreover, the number of operations was in the order of  $O((\log N)^2)$ , which was considerably lower than the complexity  $O(N \log N)$  of the Fast Fourier Transform, the quickest classical algorithm for spectral analysis.<sup>20</sup>

Second, Shor showed that the quantum Fourier transform was a tool to do phase estimation—i.e., estimating the phase  $\varphi$  of a given operator  $U$ 's eigenvalue ( $U|u\rangle = e^{i2\pi\varphi}|u\rangle$ ). The reason that the quantum Fourier transform was useful for such a task was clear: The phase estimation was equivalent to the operation of period finding, which could be done with spectral (Fourier) analysis. Shor developed a circuit constituting of Hadamard gates, a controlled-NOT gate, and a quantum Fourier transformer for the purpose of phase estimation.

Third, phase estimation was quite close to order finding, for both belonged to a general class of period-finding operations. In fact, Shor developed a formulation of the order-finding problem in terms of the phase-estimation problem. Thus, the order-finding problem was solved with a more efficient approach using quantum parallelism, since the major building block of the new approach—the quantum Fourier transform—had a significantly lower complexity than its classical counterparts.

Third, phase estimation was quite close to order finding, for both belonged to a general class of period-finding operations. In fact, Shor developed a formulation of the order-finding problem in terms of the phase-estimation problem.<sup>21</sup> Thus, the order-finding problem was solved with a more efficient approach using quantum parallelism, since the major building block of the new approach—the quantum Fourier transform—had a significantly lower complexity than its classical counterparts.

However, what was the use of solving the order-finding problem beyond satiating the curiosity of some number theorists? Shor argued that the order-finding problem could be applied to tackle two other problems with enormous practical implications: factorization of a large integer and finding the discrete logarithm of a number with respect to a cyclic group. The factorization problem seeks to obtain the factors of an integer equaling to the product of two large prime numbers, whereas the discrete logarithm problem is, roughly, to find the minimum solution  $r$  of the equation  $x^r \equiv p \pmod{N}$  for given  $x$ ,  $p$ , and  $N$ . Both problems are crucial in contemporary cryptography. The factorization of the product of two large prime numbers, for instance, has been the theoretical backbone of today's most popular public-key encryption scheme—the RSA algorithm that Ron Rivet, Adi Shamir, and Leonard Adleman developed in the 1970s. The best classical algorithm to factorize a large number  $N$  has the order of complexity no better than  $O(N^{1/3})$ , and this intractable time prevents any effective way of breaking the encrypted code. Nevertheless, Shor's quantum algorithm for factorization can achieve a complexity as low as  $O((\log N)^2 \log(\log N) \log(\log(\log N)))$ , which is improved *exponentially* over the

---

<sup>20</sup> Shor (1994), 127–128.

<sup>21</sup> *Ibid.*, 128–129.

classical algorithms. With Shor's algorithm, therefore, the security of most current communications systems is at stake.<sup>22</sup>

The quantum factorization and discrete-logarithm algorithms developed in 1994 were the first algorithms for quantum computers to solve "real-world" problems. Compared with the Deutsch-Jozsa scheme, Shor's algorithms were more "practical." Within two years, the computer scientist Lov Grover proposed another major quantum algorithm for practical applications. Like the factorization and discrete logarithm scheme, this algorithm was also originated from the Bell Laboratories.

Lov Kumar Grover was born in India. After obtaining a Bachelor's degree in Indian Institute of Technology in Delhi, he moved to the United States for further study and work. Grover once taught in the Department of Electrical Engineering at Cornell University, but later left Cornell to join the Bell Laboratories as a researcher. In the mid-1990s, he became aware of Shor's work, probably through the internal communications at the Bell Labs. The idea of using quantum characteristics in algorithm design gave him a clue to solving a problem that had concerned him—the search problem.

Searching a database is a common task in information processing and computer science. Yet this trivial work becomes extremely time consuming when the size of the database is huge. Suppose in a set of  $N$  elements there are some element  $x$  that satisfies the condition  $f(x) = 1$  (the other elements  $y$  have  $f(y) = 0$ ). The aim is to find all the  $x$ 's among the  $N$  elements. Since the entire data set does not need to have a regular structure, however, it is difficult to come up with a search scheme that saves time in general. So far, the most efficient classical algorithm is to check the elements one by one, which takes  $O(N)$  steps.

Grover got a different idea from quantum computing, though. In 1996, he proposed a quantum search scheme that would reduce the algorithmic complexity from  $O(N)$  to  $O(\sqrt{N})$ . In his own words, "quantum mechanics helps in searching for a needle in a haystack."<sup>23</sup> The central idea underlying Grover's quantum search algorithm is quantum parallelism, too. Since superposition quantum states can carry the information about the  $f(\cdot)$  values of all the elements in the data set, we may save significant time by making use of such superposition quantum states. Specifically, Grover's search algorithm begins with the preparation of a superposition state containing all the elements of the data set. Then a series of identical operations are employed on the state. The aim of these iterative operations is to "rotate" the quantum state toward the subspace corresponding to the solution  $f(x) = 1$  (Figure 3). Thus, after each iterative operation, the quantum state moves closer to the solution state. Grover showed that it takes about  $O(\sqrt{N})$  steps to align the quantum state with the solution state, the objective of the search.<sup>24</sup>

The quantum factorization, discrete-logarithm, and search algorithms developed in the 1990s marked a significant step in the history of quantum computing. Before, quantum computing was either entertained as an alternative formulation to the Turing machine model or exploited to tackle only fabricated problems. Shor's and Grover's quantum algorithms solved "real-world" problems important to pure as well as applied mathematicians. They represented the initial success—at least at the theoretical level—of

---

<sup>22</sup>Ibid, 130–133; Peter W. Shor, "Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer," *SIAM Journal of Computing*, 26 : 5 (1997), 1484–1509.

<sup>23</sup>Lov K. Grover, "Quantum mechanics helps in searching for a needle in a haystack," *Physical Review Letters*, 79 : 2 (1997), 325–328.

<sup>24</sup>Ibid, 326–328.

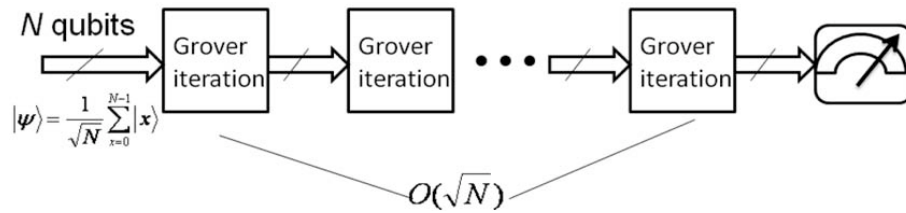


Figure 18.3: Deutsch-Jozsa Algorithm

harnessing the strange properties of quantum mechanics and turning the entanglement-like behaviors of the wave functions into valuable resources for the solution of practical problems. The introduction of the quantum factorization, discrete-logarithm, and search algorithms turned quantum computing from a confined and esoteric subject mainly interested to theoretical physicists into an active research area for mathematicians, computer scientists, and electrical engineers.

### Contemplating Quantum Communications

As physicists and computer scientists were seeking algorithms for quantum computers, another idea of quantum information was being considered. The idea was to use the strange properties of quantum mechanics in the transmission of information. Historically, the research on communications systems had a close relationship with the study of computation—the rise of modern communications engineering in the 1940–60s was owing to the revolution of digital computing, information theory and computer science had shared some common mathematical tools, both areas in the early stage were under the same disciplinary rubric of “information science,” etc. In the case of quantum communications and computing, the connection was built into the core methodology and problematics. Both exploited and manipulated the fundamental characteristics of wave functions, but with different purposes. Quantum computing aimed at developing efficient algorithms to reduce computational complexity. By contrast, quantum communications set the goal of finding information transmission schemes, or “coding,” with a higher rate, more fault tolerance, and more security. Moreover, while quantum computing utilized a broader realm of quantum phenomena such as parallelism and superposition, quantum communications relied directly on entanglement.

It is natural to connect entanglement with communications problems. The correlation between the two particles of an entangled pair had invited attempts to devise information-transmission schemes. Since Einstein, Podolsky, and Rosen, scholars had disputed about whether information transmission based on the entangled state would lead to unlawful consequences such as superluminal action or time reversal. Yet, most discussions on this topic before the 1970s focused on the consistency and completeness of quantum mechanics. A pioneering effort to turn entanglement into communications resource was made by the American researcher Charles Bennett.

Charles Bennett was a native of Massachusetts. He obtained B.S. from Brandeis University in 1964 and Ph.D. from Harvard University in 1970, both in chemistry. Bennett’s training was physical chemistry; he conducted doctoral dissertation project concerned molecular dynamics. After graduation, he spent two years as a postdoc at Argonne Lab-

oratory and eventually took a position at the IBM Research Center in New York State in 1972. At the time, the IBM Research was a center for exploring cutting-edge computers. For instance, the Corporation had invested on the research into superconducting logical circuits as a hopeful candidate for the computers of the next generation. Rolf Landauer had also established his research group on the physics of computation at IBM. When Bennett joined IBM, he worked under Landauer, who changed his interest from molecular dynamics to the relationship between physics and information. In the 1970s and early 1980s, Bennett contributed to various subjects in the physics of computation, including the formulation of a reversible universal computer and a reinterpretation of “Maxwell’s demon” in the context of computation.<sup>25</sup>

Bennett began to pay close attention to entanglement in the early 1980s. The recent success of realizing the EPR experiment in laboratory<sup>26</sup> gave him the motivation of using the entangled states in communications. Bennett’s first thought was quantum cryptography, the application of quantum characteristics to encrypting messages. This idea had existed for a while. In the 1970s, a physics student Stephen Wiesner at Columbia University had thought of certain “quantum money” that could withstand counterfeit.<sup>27</sup> Wiesner’s proposal was not taken seriously, but Bennett’s was. In 1982–84, he collaborated with the computer scientist Gilles Brassard in the Département d’Information et de Recherche Opérationnelle at Université de Montréal to develop a scheme of quantum cryptography. The key principle of this scheme is that the quantum state of a particle is changed permanently after a measurement. Suppose a person sends a message coded into, say, the polarized state of a photon, to another person. If an eavesdropper is trying to tap this message, then he has to make a measurement of the photon’s state, which changes it permanently.

Consequently, the received message differs from the sent message. With some protocol that the sender and the recipient exchange via another non-quantum channel, such a discrepancy can be detected. And since this discrepancy marks eavesdropping, both parties can drop the message of concern. In general, this procedure guarantees only the non-eavesdropped messages to get through. Encryption upholds!<sup>28</sup> With the help of Bennett colleague John Smolin, Bennett and Brassard supervised the building of an experimental demonstration for quantum cryptography at IBM in 1989.<sup>29</sup>

Bennett and Brassard’s quantum cryptographic protocol applied quantum principles to protect the security of communications. More fundamentally, they had shown that

---

<sup>25</sup><http://www.research.ibm.com/people/b/bennetc/chbbio.html>.

<sup>26</sup>Alain Aspect, Phillipe Grangier, and Gérard Roger, “Experimental realization of Einstein-Podolsky-Rosen-Bohm Gedanken Experiment: a new violation of Bell’s inequalities,” *Physical Review Letters*, 49 : 2 (1982), 91–94; Alain Aspect, Jean Dalibard, and Gérard Roger, “Experimental tests of Bell’s inequalities using variable analysis,” *Physical Review Letters*, 49 : 25 (1982), 1804–1807; M.A.Horne and Anton Zeilinger, “Einstein-Podolsky-Rosen interferometry, new techniques and ideas in quantum measurement theory,” D.Greenberger (ed.), *Annals of the New York Academy of Sciences*, 480 (1986), 469.

<sup>27</sup>Stephen Wiesner, “Conjugate coding,” *SIGACT News*, 15 (1983), 77.

<sup>28</sup>Charles H. Bennett and Gilles Brassard, “Quantum Cryptography: Public Key Distribution and Coin Tossing,” *Proceedings of IEEE International Conference on Computers Systems and Signal Processing, (Bangalore India, December 1984)* 175–179.

<sup>29</sup><http://www.research.ibm.com/people/b/bennetc/chbbio.html>; Charles H. Bennett and Gilles Brassard, “The dawn of a new era in quantum cryptography: the experimental prototype is working,” *ACM SIGACT News*, 20 (1989), 78–83.

one might use quantum states of particles as particular “channels” for information transmission; for instance, one could code the information into the polarized states of photons and send out the photons as information carrier. What are the characteristics of such quantum channels? In addition to encryption, what are the advantages of employing the quantum channels? Can they help increase the rate of information transmission, arguably the primary *raison d’être* of communication engineering? In the early 1990s, Bennett and his collaborators discovered a few interesting ways of manipulating the EPR states that offered clues to answer the above questions. Specifically, they found means to appropriate entanglement in implementing effective information-transmission systems.

The first finding came in 1992. Bennett and Stephen Wiesner suggested that a specific way of manipulating an EPR state led to a high-rate information transfer. Later known as “superdense coding,” Bennett and Wiesner’s scheme worked as follows (Figure 4): Suppose Alice wants to send a two-bit piece of information to Bob, who is far away from her. Either Alice or Bob or a third person prepares a two-particle entangled state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle|0\rangle + |1\rangle|1\rangle) \tag{18.2}$$

(Note this state is different from the one Bohm and Bell used in (1). Yet both states exhibit the perfect correlation between the two particles that the EPR condition demands.) Now, deliver the first qubit of  $|\psi\rangle$  to Alice and the second qubit to Bob. Since both qubits are from the same EPR state, they should have a perfect correlation even though they are possessed by two individuals far apart. After each of them obtains the respective qubit, Alice performs one of the four operations on the qubit she gets, and these operations can be numerated with two binary numbers:

00	no operation	$\alpha 0\rangle + \beta 1\rangle \mapsto \alpha 0\rangle + \beta 1\rangle$
01	phase flip	$\alpha 0\rangle + \beta 1\rangle \mapsto \alpha 0\rangle - \beta 1\rangle$
10	state swap	$\alpha 0\rangle + \beta 1\rangle \mapsto \beta 0\rangle + \alpha 1\rangle$
11	phase flip+state swap	$\alpha 0\rangle + \beta 1\rangle \mapsto \beta 0\rangle - \alpha 1\rangle$

The operation Alice performs on her qubit depends on the message she intends to send to Bob: If she wants to send 00, then she leaves the qubit intact; if she wants to send 01, then she performs phase flip, etc. After the operation, Alice sends the qubit to Bob via a quantum channel. Upon receiving Alice’s qubit, Bob possesses two entangled particles with the overall quantum state having one of the four possibilities:

00	$ \phi\rangle = \frac{1}{\sqrt{2}}( 00\rangle +  11\rangle)$	
01	$ \phi\rangle = \frac{1}{\sqrt{2}}( 00\rangle -  11\rangle)$	
10	$ \phi\rangle = \frac{1}{\sqrt{2}}( 10\rangle +  01\rangle)$	
11	$ \phi\rangle = \frac{1}{\sqrt{2}}( 01\rangle -  10\rangle)$	(3)

Since the states in (3) are orthogonal to each other, Bob can devise a measuring instrument to distinguish  $|\phi\rangle$  perfectly among the four possibilities. By measuring the quantum state of the two entangled particles, therefore, Bob can figure out whether Alice sends 00, 01, 10, or 11, meaning that he is able to retrieve the information Alice transmits. Moreover, the transmission of this *two-bit* information is achieved with the



communication of only one qubit from Alice to Bob. In other words, the rate of information transmission is doubled using EPR and the quantum channel! In 1992, Bennett and Wiesner published their scheme in *Physical Review Letters*.<sup>30</sup>

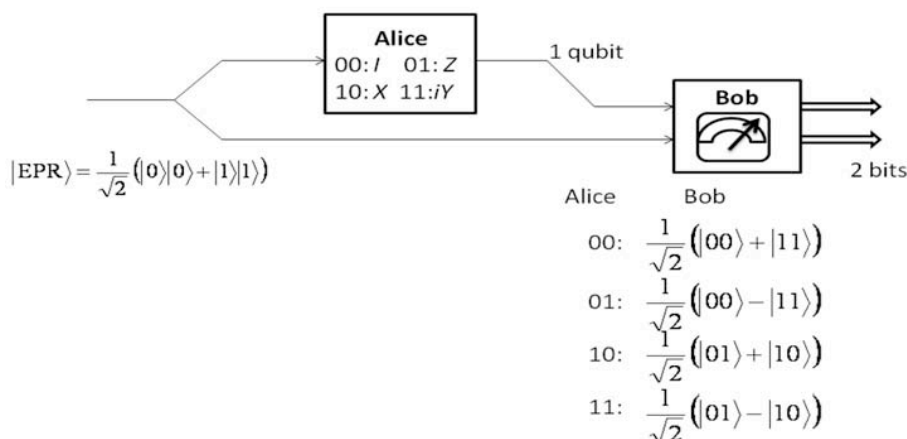


Figure 18.4: Superdense Coding

Bennett and Wiesner’s proposal turned out to be only the first step toward a more unintuitive result in quantum communications. In the 1992 paper, they pointed out that the essence of their scheme was to split the two qubits of an EPR pair, manipulate a qubit at one side, and return the result of manipulation in some way to the other side. The superdense coding was just a special case of a more generic procedure like that. The paper also discussed the conditions in which some “ancilla,” an additional quantum state, was coupled with one qubit of the EPR pair. The incorporation of the ancilla gave the communications system more freedom to manipulate, which facilitated the production of more novel effects. An immediate one was “quantum teleportation,” the faithful transport of a quantum state from one place to another.

The work on quantum teleportation in 1993 resulted from a multinational collaboration involving the U.S., Canada, Israel, and France. The participants included Bennett, Brassard, Brassard’s colleagues Claude Crépeau (who was also affiliated with the École Normale Supérieure in Paris) and Richard Jozsa at the Université de Montréal (Jozsa had moved to Montréal in 1985), Asher Peres at Technion-Israel Institute of Technology, and William Wootters at Williams College.<sup>31</sup> Their starting point was the longstanding question whether the long-range correlation between the two elements of an EPR pair can be used in information transfer. Since Einstein, scholars had focused on resolving any scenario that might violate the laws of physics. An example is the demonstration that instantaneous information transfer is impossible with an EPR pair, which saves the premise of relativity that nothing travels faster than light. Yet, Bennett *et al.* were not concerned with the meta-theoretical problems of compromising EPR with existing

<sup>30</sup>Charles H. Bennett and Stephen J. Wiesner, “Communication via one- and two-particle operators on Einstein-Podolsky-Rosen states,” *Physical Review Letters*, 69 : 16 (1992), 2881–2884.

<sup>31</sup>C.H. Bennett, G. Brassard, C. Crépeau, R. Jozsa, A. Peres, and W. Wootters, “Teleporting an Unknown Quantum State via Dual Classical and Einstein-Podolsky-Rosen Channels,” *Physical Review Letters* 70 : 13 (1993), 1895–1899.

physical laws. Instead, they were interested in what can be done with entanglement. Although the EPR state cannot be used to perform instantaneous information transfer, they argued, it can facilitate perfect transmission, or more precisely, a faithful reproduction, of a quantum state. Here is the scheme of Bennett *et al.* to achieve quantum teleportation (Figure 5).

Suppose two far separated individuals Alice and Bob share an EPR pair. Like the case of superdense coding, Alice possesses one qubit while Bob owns the other qubit of the entangled state  $|EPR\rangle = \frac{1}{\sqrt{2}}(|0\rangle|0\rangle + |1\rangle|1\rangle)$ . Alice's task is to transmit to Bob a quantum state  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$  that she possesses but does not have any knowledge of (i.e., she does not know the values of  $\alpha$  and  $\beta$ ). To achieve this end, Alice interacts her qubit of the EPR pair with the unknown quantum state  $|\psi\rangle$ . Her exact operations consist of a controlled-NOT gate taking  $|\psi\rangle$  as the controlled qubit and a Hadamard gate on  $|\psi\rangle$ . Although these gates operate on  $|\psi\rangle$  and Alice's qubit of  $|EPR\rangle$ , they modify the joint quantum state of  $|\psi\rangle$  and  $|EPR\rangle$ , because Bob's EPR qubit and Alice's EPR qubit are perfectly correlated. After simple quantum mechanical calculations, it can be shown that the resultant joint state is the superposition of four distinct terms: Alice's qubits are  $|00\rangle$  while Bob's qubit is  $\alpha|0\rangle + \beta|1\rangle$ , Alice's qubits are  $|01\rangle$  while Bob's qubit is  $\alpha|1\rangle + \beta|0\rangle$ , Alice's qubits are  $|10\rangle$  while Bob's qubit is  $\alpha|0\rangle - \beta|1\rangle$ , Alice's qubits are  $|11\rangle$  while Bob's qubit is  $\alpha|1\rangle - \beta|0\rangle$ . This result indicates that Bob now possesses all the information needed to reconstruct  $|\psi\rangle$ , and he can do so as long as he knows the exact state of Alice's qubits. So Alice's next step is to measure her two qubits to see whether the outcome  $M_1M_2$  is 00, 01, 10, or 11. Then she transmits these two classical bits  $M_1$  and  $M_2$  via a classical channel to Bob. Upon receiving  $M_1$  and  $M_2$ , Bob decides which operation to take against his qubit: no action at all for 00, a state swap for 01, a phase flip for 10, a state swap and a phase flip for 11. In all the four conditions, Bob's qubit output is guaranteed to be  $\alpha|0\rangle + \beta|1\rangle$ , a faithful reproduction of the original  $|\psi\rangle$ .

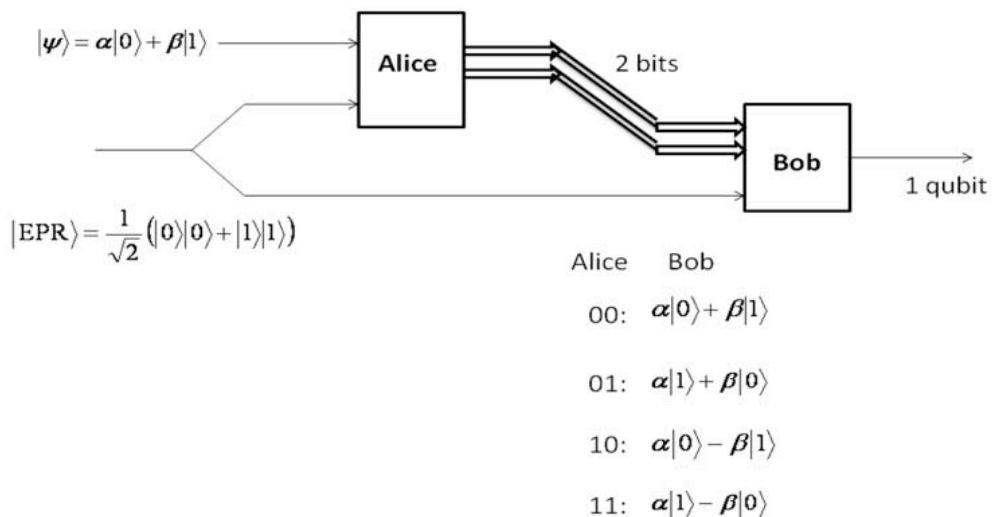


Figure 18.5: Quantum Teleportation

The quantum teleportation provides a prototypical case for quantum communications.

Its arrangement exhibits certain important features common to a lot of more sophisticated quantum communication schemes. First, entanglement is the crucial resource for the system. The protocol of the system starts with two communicative parties sharing different elements of an EPR pair. Often the message is coded on a separate quantum state rather than an EPR qubit. Yet the message state has to “interact” with the EPR qubit in some algorithmic manner in order to exploit EPR’s correlation property. Second, the access to the quantum information is a tricky issue. Unlike classical information processing, the transmitter and receiver of a quantum communications system cannot freely copy a message or read a message without disturbing it. In the case of teleportation, for instance, Alice does not have any knowledge of the information she sends to Bob. Nor can she keep a copy of the message state afterwards, for the message state is collapsed after the measurement. Carefully designed, quantum-algorithmic-like operations are necessary in the management of information flow. Finally, “classical” channels may play an important part in quantum communications. Sometimes a quantum channel has to be augmented with conventional digital transmission in order to take full advantage of entanglement.

### Quantum Information: What’s Next?

From the 1980s to the mid-1990s, the pioneering works of Deutsch, Jozsa, Shor, Grover, Bennett, Brassard, Wiesner, and a few others had opened up the field of quantum information. The Deutsch-Jozsa, factorization, discrete logarithm, and search algorithms showed the promise of quantum parallelism in tackling computational problems. The ideas of quantum cryptography, superdense coding, and teleportation demonstrated the potential of entanglement in communications engineering. By the beginning of the twenty-first century, quantum information science had become a cutting-edge area with many participants from diverse disciplines and all parts of the world. An online “who’s who” for quantum information science features more than two hundred scholars from North America and Europe as well as East Asia, Middle East, and Latin America. The people studying quantum information had expanded into a significant, international community. What are their research agendas? What do they try to do? What is the next after the surge of innovations in the 1980s–90s?

Physical realizations of quantum computers and quantum communications systems have been a primary concern for those working in this area. Deutsch and Jozsa’s, Shor’s, and Grover’s algorithms, as well as Bennett et al.’s EPR-related communications protocols existed only on papers when they were proposed. Since the 1990s, physicists and engineers have tried to implement these ideas in laboratories. It would be a daunting task to trace the numerous experimental endeavors on quantum information in this paper. Suffice to observe that the implementation of quantum computers and communication systems has been built upon a different set of knowledge and skills from conventional computer engineering, electronic engineering, and material science. Unlike the computers and electronics we are using today, quantum computers and communications systems are difficult to realize using semiconductor materials. In fact, the making of these quantum information devices seems to concern not the choice and engineering of specific materials, but the ability to manipulate single atoms and photons and prepare pure quantum states. Thus, atomic physics and optoelectronics have played more important parts in quantum information experiments than condensed-matter physics and

semiconductor electronic engineering.

The first notable success of quantum information experiments came from the physical implementation of simple quantum communications schemes. In 1996, researchers at the Universität Innsbruck in Austria and Los Alamos National Laboratories reported production of the superdense coding phenomenon in laboratory. In 1997–98, the Innsbruck group, and the research teams at the Università Roma, Italy, and Caltech succeeded in the experimental realization of quantum teleportation.<sup>32</sup> All these physicists used photons (more specifically, laser) in their implementation of quantum communication schemes. The choice of laser had good historical reasons: After the invention of laser in the 1960s and the development of optical fibers in the 1970s, optoelectronics had become a major means of high-bandwidth digital communications. In the process of designing efficient fiber networks, optoelectronic engineers and applied physicists had accumulated rich knowledge and skills in preparing and handling pure quantum states of photons such as the coherent state and the squeezed state. These became handy techniques for the experimenters working on EPR. In fact, the first successful laboratory productions of the EPR pairs in the early 1980s were accomplished by atomic physicists using laser apparatus. By the 1990s, therefore, the EPR photon-pair generator consisting of beam splitters and nonlinear parametric amplifiers had become an available device for the quantum information experimenters.

Although optoelectronics may be an effective way of implementing quantum communications systems, its applications in quantum computers have encountered some problems. Some have argued that photons are more difficult to interact with and to store than atoms, so a more feasible quantum computer should be made of the latter. In the mid-1990s, researchers proposed to use trapped ions to implement quantum computers. A technique invented in the 1970s by the German atomic physicists Hans Dehmelt and Wolfgang Paul, respectively, the ion trap utilized an electromagnetic field to confine charged particles within a small volume.<sup>33</sup> The ion trap was originally adopted to the studies of atoms or smaller elementary particles, and hence were more familiar to atomic physicists and particle physicists. This technique was brought to quantum computing, because it offered means to prepare and manipulate atomic particles at simple quantum states. Another popular candidate for the physical implementation of quantum computers is Nuclear Magnetic Resonance (NMR). NMR was another product of the mid-century boom of atomic physics (like laser and ion traps). Chemists and biomedical engineers had spent decades to elaborate and improve the device; by the 1990s, it had become a mature laboratory technology. Since a proposal in 1995, the NMR quantum computer has attracted much attention of quantum information scientists. The major advantage of NMR over ion traps or laser is that NMR functions at the macroscopic level: the data is registered at thousands or even millions of spinning nuclei instead of a few atoms or photons. But this advantage is also NMR's serious shortcoming: it is much more difficult to control the quantum state of a sea of spinning nuclei than that of several

---

<sup>32</sup>D. Bouwmeester, J.W. Pan, K. Mattle, M. Eibl, H. Weinfurter, and A. Zeilinger, "Experimental quantum teleportation," *Nature*, 390 : 6660 (1997), 575–579; D. Boschi, S. Branca, F. De Martini, L. Hardy, and S. Popescu, "Experimental realization of teleporting an unknown pure quantum state via dual classical and Einstein-Podolsky-Rosen channels," *Physical Review Letters*, 80 : 6 (1998), 1121–1125; A. Furusawa, J.L. Sørensen, S.L. Braunstein, C.A. Fuchs, H.J. Kimble, and E.S. Polzik, "Unconditional quantum teleportation," *Science*, 282 (1998), 706–709.

<sup>33</sup>[http://nobelprize.org/nobel\\_prizes/physics/laureates/1989/index.html](http://nobelprize.org/nobel_prizes/physics/laureates/1989/index.html).

atoms or photons. Recently, quantum information scientists have also proposed to extend the candidacy to superconductors, quantum dot, and ordinary semiconductors. But none of these approaches—including optoelectronics, ion traps, and NMR—has reached the stage of practicality. To date, there has not yet been a quantum computer with more than a few qubits, let alone a machine with sufficient qubits indispensable to realize the strength of the factorization, discrete logarithm, and search algorithms.

A major problem for the physical implementation of quantum computers and communications systems is noise. A single, coherent quantum state is very easy to collapse by a slight interaction with its environment. While experimenters' challenge is to maintain the purity of quantum states and remove the sources of noise, theorists' task is to develop algorithms, schemes, and protocols that are more robust to noise. Since the mid-1990s, much of the theoretical work on quantum information science has focused on this issue. Shor's factorization algorithm, Grover's search scheme, and Bennett *et al.*'s superdense coding, for instance, all perform well in an idealized world. But how would they function in the real, noise-infected world? Can we find ways to save their performance with the presence of disturbance? A popular topic among quantum information scientists is quantum error-correction codes. Peter Shor in 1995 and Andrew Steane of Oxford University in 1996 respectively devised error-correction codes for qubits. Similar to classical error-correction codes, their approaches were to interact the data qubits and some redundant qubits with quantum operations equivalent to parity check.<sup>34</sup> The ideas of quantum error-correction coding inspired theoretical works along several directions: In quantum computing, it led to the development of fault-tolerant computing gates that guarantee at least some degrees of performance for quantum algorithms in a noisy environment.

In quantum communications, the similarity between quantum error-correction codes and classical error-correction codes has encouraged theorists to construct a comprehensive quantum communications science analogous to the existing classical communications science. The most important development has been the building of a quantum information theory parallel to the Shannon-like information theory. Like Shannon's followers, the quantum information theorists are seeking the capacity of a quantum channel and consequently the best possible performance of a quantum communication system. They are also looking for the applications of the knowledge about channel capacity to the efficient design of error-correction, data-compression, and cryptographic codes. As of 2007, scholars believe that they still know "only a little of quantum information theory."

Quantum information devices are not yet a reality, if not an impossibility. Despite conspicuous financial support from NSF, DARPA, and other major funding agencies around the world, they remain research ideas and crude experimental prototypes that at best show uncertain promises.<sup>35</sup> Will there eventually be quantum computers or communications systems? Is the entire field a hype or hope? Although our task is not to

---

<sup>34</sup>A famous example is Peter Shor, "Fault-tolerant quantum computation," *Proceedings of the 37th Annual Symposium on Foundations of Computer Science* (1996), 56–65. Also see Nielsen and Chuang (2000), 425–499.

<sup>35</sup>Rolf Landauer, IBM's chief physicist of computation considered by many as a godfather of quantum computation, once suggested that all papers on quantum computing should carry a footnote: "This proposal, like all proposals for quantum computation, relies on speculative technology, does not in its current form take into account all possible sources of noise, unreliability and manufacturing error, and probably will not work." Seth Lloyd, "Obituary: Rolf Landauer (1927–99)," *Nature*, 400 : 6746 (1999), 720.

answer these questions, we can nonetheless observe from such questions what kind of pursuit have the studies of quantum information become. In this paper, I trace how the research into the foundation of quantum mechanics has evolved into an expanded technological project. The process started with physicists/philosophers' epistemological and ontological questions about entanglement, non-locality, and interference—what they are, how to understand them, *etc.* Gradually, however, the central research agendas were amended to pragmatic questions such as how to produce, manipulate, and make use of them. With the introduction of specific quantum algorithms and quantum communications protocols, entanglement and related properties had been turned from puzzles to be explained into resources for information processing. Engineering entanglement has become equally important to, if not dominated over, pondering the interpretation of quantum mechanics. Does this epistemic transformation indicate that quantum mechanics has reached a mature stage so that we stop worrying about its conceptual foundation and feel comfortable using it? I don't know. But I believe this story tells us as much about the technological nature of today's scientific practice as about our understanding of quantum mechanics.