# Erwin Schrödinger and the Rise of Wave Mechanics.<sup>1</sup> III. Early Response and Applications

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This article (Part III) deals with the early applications of wave mechanics to atomic problems—including the demonstration of the formal mathematical equivalence of wave mechanics with the quantum mechanics of Born, Heisenberg, and Jordan, and that of Dirac—by Schrödinger himself and others. The new theory was immediately accepted by the scientific community.

# **13. THE SCHEME STARTS TO WORK**

In his letter of January 29, 1926 to Sommerfeld, Schrödinger, after referring to his first communication (on the hydrogen atom), mentioned: "I have since translated a few further mechanical problems into the conceptual scheme. As far as my mathematical methods suffice, everything develops in the nicest way; and it is still *not* a stereotype of the old quantum rules, but differs from it in characteristic points."<sup>(311)</sup> He then explained in a few sentences the results: (i) on the linear oscillator; (ii) on the rotator in three dimensions; and (iii) on the free motion of a mass point. Finally, he stated the problems that had to be treated next in the new theory, i.e., "besides the evaluation of important special cases—like the Stark effect, the Zeeman effect, and the relativistic Kepler motion—the establishment of a rule for the intensity and polarization which must replace the correspondence

<sup>&</sup>lt;sup>1</sup> This article (in three parts) is an expanded version of the Schrödinger Centenary Lecture delivered by me at CERN (Organisation Européenne pour la Recherche Nucléaire), 1211 Geneva 23, Switzerland, on July 30, 1987.

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principle."<sup>(311)</sup> He had already begun the investigation of parts of these problems and would complete and publish them in the following months. The results constituted the first tests and confirmation of the theory of wave mechanics, which had originally been derived for the specific case of calculating the energy states of the hydrogen atom.

# 13.1. The Oscillator in Wave Mechanics

The most important content of undulatory or wave mechanics could be expressed in the form of the general, second-order differential equation,

div grad 
$$\psi + \frac{8\pi^2}{h^2} (E - V) \psi = 0$$
 (113)

for the wave function  $\psi$  describing atomic systems of arbitrarily many degrees of freedom. Equation (113) took on a well-defined shape, if the potential energy V of the system was given as a function of, say, its f position and f momentum or velocity coordinates. The differential operation "div grad" had to be interpreted as operating in an f-dimensional Riemmannian space, with the line element

$$ds^2 = 2\bar{\mathfrak{J}}(q_k, \dot{q}_k) dt^2 \tag{114}$$

where  $\bar{\mathfrak{I}}$  denoted the kinetic energy of the system when expressed as a function of the position and velocity coordinates,  $q_k$  and  $\dot{q}_k$ , k = 1, ..., f.

In figuring out the applications of wave mechanics beyond the nonrelativistic hydrogen problem and the hydrogen atom in a magnetic field, Schrödinger soon alighted on the problem of the linear oscillator.<sup>(312)</sup> This problem had played a distinguished role in the history of quantum theory, because it was the quantization of the linear oscillator that provided the starting point for the entire theory. Schrödinger also knew that the result of any new treatment of the oscillator had to coincide more or less with the one presented by Max Planck as early as December 1900; it had especially to yield the famous, repeatedly substantiated blackbody radiation law. Whether this result would be obtained by the wave mechanical method could not be considered as being obvious; hence, even the solution of a problem as simple as the one-dimensional linear oscillator provided a crucial test of the new scheme, in which the quantization was not imposed directly but rather followed via applying boundary and uniqueness conditions on the wave function satisfying Eq. (113) in that special case.

Evidently, in the case of the one-dimensional linear oscillator, the kinetic energy  $\bar{\mathfrak{Z}}$  could be written as

$$\overline{\mathfrak{Z}} = \frac{1}{2}\dot{q}^2 \tag{115}$$

provided the single position coordinate q was chosen to be the elongation times the square-root of the oscillating mass. From Eq. (114) it then followed immediately that the line element, i.e.,

$$ds^2 = \dot{q}^2 dt^2 \tag{116}$$

defined a (one-dimensional) Euclidean space. As a consequence, the second-order derivative term in Eq. (113) simply redued to the second-order derivative with respect to q, hence

div grad 
$$\psi = \frac{d^2 \psi}{dq^2}$$
 (117)

Further, the potential energy V depended only on the position variable q and the oscillator frequency  $v_0$ , that is,

$$V(q) = 2\pi^2 v_0^2 q^2 \tag{118}$$

On inserting Eqs. (117) and (118) into Eq. (113), Schrödinger arrived at the equation

$$\frac{d^2\psi}{dq^2} + (a - bq^2)\psi = 0$$
(119)

with

$$a = \frac{8\pi^2 E}{h^2} \tag{119a}$$

and

$$b = \frac{16\pi^4 v_0^2}{h^2} \tag{119b}$$

to describe the one-dimensional linear oscillator in wave mechanics.

In his notebook on "*Eigenwertproblem des Atoms. I*" (on p. 45), Schrödinger had indicated how to transform Eq. (119) into the Laplacian equation

$$\frac{d^2\psi}{dx^2} + \frac{1}{2x}\frac{d\psi}{dx} + \left(\frac{a}{4x} - \frac{b}{4}\right)\psi = 0$$
(120)

by means of the transformation

$$q^2 = x \tag{121}$$

Equation (120) had basically the same form as the one describing the Kepler problem; he then wrote down the solution along the lines which had worked before in the case of the nonrelativistic hydrogen atom. He immediately added that the very same solution followed from another, rather different path, if one transformed Eq. (119) into the differential equation for the Hermitian orthogonal functions, referring at this point to Courant and Hilbert's Methoden der mathematischen Physik.<sup>(313)</sup> In the published paper, i.e., the second communication on "Ouantisierung als Eigenwertproblem," he suppressed the first step and presented only the solution according to Courant and Hilbert.<sup>(314)</sup> However, at a later point in his paper. Schrödinger recalled his original solution in a footnote, in which he wrote: "Moreover, the one-dimensional oscillator leads to the same equation [i.e., a Laplacian equation similar to the one for the hydrogen atom ] if  $q^2$  is taken as variable. I originally solved the problem directly in that way. For the hint that it was a question of Hermite polynomials, I have to thank Herr E. Fues."<sup>(315)</sup>

The "equation for Hermitian polynomials" mentioned by Schrödinger was of course

$$\frac{d^2y}{dx^2} + (1 - x^2)y + \lambda y = 0$$
(122)

an equation quoted in *Courant–Hilbert* (on p. 261, the page quoted by Schrödinger in *Notebook I*, p. 45, and in the paper—Ref. 256—on p. 515), together with its complete set of continuous and (in the entire region  $-\infty \le q \le +\infty$ ) finite solutions, y(x), the Hermitian orthogonal functions  $\exp(-x^2/2) H_n(x)$ , each of which is associated with one of the proper eigenvalues  $\lambda = 0, 2, 4, 6, \dots$ .<sup>(316)</sup> The wave equation (119) for the one-dimensional linear oscillator assumed the form of Eq. (122) after the transformation of the position coordinate, namely

$$x = q\sqrt[4]{b} \tag{123}$$

Then Schrödinger obtained the new equation

$$\frac{d^2}{dx^2} + (1 - x^2)\psi + \left(\frac{a}{\sqrt{b}} - 1\right)\psi = 0$$
(124)

which implied the condition for the eigenvalues:

$$\lambda = \left(\frac{a}{\sqrt{b}} - 1\right) = 0, 2, 4, 6,\dots$$
(125)

or

$$\frac{a}{\sqrt{b}} = 1, 3, 5, \dots, 2n \pm 1 \tag{126}$$

In his published paper, Schrödinger also immediately copied from *Courant-Hilbert* the general formula for the Hermitian polynomials, i.e.,

$$H_n(x) = (-1)^n \exp(x^2) \frac{d^n \exp(-x^2)}{dx^2}$$
(127)

and the equations for the first five polynomials, i.e.,

$$H_0(x) = 1, H_1(x) = 2x$$
  

$$H_2(x) = 4x^2 - 2 H_3(x) = 8x^2 - 12x (128)$$
  

$$H_4(x) = 16x^4 - 48x^2 + 12$$

[see Ref. 256, p. 515, Eqs. (27) and (27"), and Ref. 313, p. 76, Eqs. (59) and (63)].

All that he had to do after that step, in order to find the eigenvalues of the one-dimensional linear oscillator in wave mechanics, was to insert the expressions (119a) and (119b) into Eq. (126). This yielded the result

$$E_n = \frac{(2n+1)}{2} h v_0, \qquad n = 0, 1, 2, \dots$$
 (129)

whereupon Schrödinger commented in his publication: "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  $hv_0/2$ . The intervals between the levels, which alone are important for the radiation, are the same as in the former theory."<sup>(317)</sup>

The agreement of the result for the energy eigenvalues of the onedimensional linear oscillator with the existing empirical tests satisfied Schrödinger immensely. However, he was still more ambitious, because his solutions of the wave equation (124) still contained additional information in the wave functions  $\psi_n$ , which were given by the expressions

$$\psi_n(q) = \exp\left(-\frac{2\pi^2 v_0 q^2}{h}\right) H_n\left(2\pi q \sqrt{\frac{v_0}{h}}\right), \qquad n = 0, 1, 2, 3, \dots \quad (130)$$

as functions of the position variable q. From the explicit formulas, given in *Courant–Hilbert* for Hermite polynomials,  $H_n(x)$ , Schrödinger could derive several conclusions, if he evaluated them numerically.<sup>(318)</sup> This he did in a

set of notes, entitled "Oszillatorschwingungen" ("Oscillator Vibrations"); he especially calculated the roots, maxima, and minima of several polynomials.<sup>(319)</sup> Schrödinger found the classical amplitude of the *n*th vibration to be

$$q_n = \frac{\sqrt{E_n}}{2\pi v_0} = \frac{1}{2\pi} \sqrt{\frac{h}{v_0}} \sqrt{\frac{2n \pm 1}{2}}$$
(131)

He wrote down this equation, without justifying it, in the second communication of Feburary 1926. Several months later, however, Schrödinger presented full details in a note entitled "Der stetige Übergang von der Mikro- zur Makromechanik" ("The Continuous Transition from Microto Macro-Mechanics"), which he submitted to Naturwissenschaften.<sup>(320)</sup> In this note he especially demonstrated "in concreto the transition to macroscopic mechanics, by showing that a group of eigenvibrations of high order-number n ('quantum number') and of relatively small order-number differences ('quantum number') may represent a 'particle' which is executing the 'motion,' expected from the usual mechanics, i.e., oscillating with the frequency  $v_0$ ."<sup>(321)</sup>

# 13.2. The Rotator and the Diatomic Molecule in Wave Mechanics

Immediately after treating the linear oscillator, Schrödinger started out with what he called "the simplest conceivable example of vibration theory"<sup>(322)</sup>: the rotator having an axis fixed in space. It corresponded, on the one hand, to a one-dimensional problem, hence the line-element was, of course, Euclidean in the angle  $\phi$ . On the other hand, it involved no potential energy at all. Consequently the equation of vibration, or the wave equation, assumed the form,

$$\frac{1}{A}\frac{d^2\psi}{d\phi^2} + \frac{8\pi^2 E}{h^2}\psi = 0$$
(132)

where A denoted the moment of inertia. Equation (132) evidently possessed the solution

$$\psi = \begin{cases} \sin\left(\sqrt{\frac{8\pi^2 EA}{h^2}}\phi\right) \\ \cos\left(\sqrt{\frac{8\pi^2 EA}{h^2}}\phi\right) \end{cases}$$
(133)

The boundary condition, demanding the uniqueness and the continuity of the solution throughout the entire range of the angle  $\phi$ , led to the equation

$$E_n = \frac{n^2 h^2}{8\pi^2 A} \tag{134}$$

with *n* assuming integral values<sup>(323)</sup></sup>

$$n = 0, 1, 2, 3, \dots$$
 (134a)

By Eq. (134) the energy values of the rotator were restricted to a discrete sequence, as was formerly the case through the quantization rule in the Bohr–Sommerfeld theory of the same system, which had been suggested—even before Bohr and Sommerfeld—by Paul Ehrenfest.<sup>(324)</sup> One had also tried to discuss physical examples of microscopic rotating systems; thus one associated energy difference from Eq. (134) with the band spectra or the specific heats of diatomic molecules, achieving rather mixed success. Schrödinger now declared frankly: "No meaning, however, can be attached to the result of the application to band spectra.... It is a peculiar fact that our theory gives *another* result for the rotator with *free* axis. *And this is true in general.* It is not allowable in the applications of wave mechanics, to think of the freedom of movement of the system as being more strictly limited, in order to simplify calculation, than it actually is, even when we know from the integrals of the mechanical equations that in a single movement certain definite freedoms are not made use of."<sup>(325)</sup>

While a diatomic molecule could not, even in a weak approximation, be represented by a rigid rotator with *fixed* axis, a rigid rotator with *free* axis may be considered a suitably simplified model of the atomic system. Schrödinger discussed such a model in his paper, where he used the two polar angles,  $\theta$  and  $\phi$ , made by the line connecting the two nuclei (of the molecule), as position variables. In those variables and their canonically conjugate (angular) momenta,  $p_{\theta}$  and  $p_{\phi}$ , the kinetic energy was expressed as

$$\Im = \frac{1}{2A} \left( p_{\theta} + \frac{p_{\phi}^2}{\sin^2 \theta} \right)$$
(135)

Equation (135) also described the kinetic energy of a point particle whose motion is constrained to a spherical surface. The Laplacian operator  $\Delta$  in the fundamental equation (113), therefore, can be identified in this case with that part of the spatial Laplacian operator in the spherical coordinates, r,  $\theta$ , and  $\phi$ , which depends only on the polar angles, i.e.,

$$\Delta = \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left( \sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2}$$
(136)

Finally, the wave equation for the rigid rotator with free axis becomes rather similar to Eq. (132), i.e.,

$$\frac{1}{A}\Delta\psi + \frac{8\pi^2 E}{h^2}\psi = 0$$
(137)

Due to the different structure of the Laplacian operator, however, the wave mechanical boundary conditions yielded the eigenvalue equation

$$\frac{8\pi^2 A}{h^2} E = n(n+1)$$
(138)

with

$$n = 0, 1, 2, 3, \dots$$
 (138a)

or the energy levels

$$E_n = \frac{n(n+1)h^2}{8\pi^2 A}, \qquad n = 0, 1, 2, 3,...$$
(139)

Schrödinger realized immediately that the result, Eq. (139), deviated from *all* results of the old quantum theory. However, he also noticed that "various arguments from experiment ... led to putting 'half-integral' values for *n* in formula (134)."<sup>(326)</sup> Indeed the use of half-integral quantum numbers in the old quantum-theoretical rotator formula provided practically the same result as Eq. (139), because the identity

$$n(n+1) = (n+\frac{1}{2})^2 - \frac{1}{4}$$
(140)

reduced the discrepancy between the energy values given by Eqs. (134) and (139), respectively, to—in general—the small additional term  $\frac{1}{4}$ . The practical identity of the wave mechanical result for the rotator with free axis, and the result derived from the old quantization rules with half-integral quantum numbers, could even be shown to be valid in the case of the short-wave bands as well, where electronic jumps resulted in different moments of inertia for the initial and final state of the molecule. For that purpose, Schrödinger discussed, in the last part of his second communication, a more realistic model of a diatomic molecule.<sup>(327)</sup>

# 13.3. The Transcription of Epstein's Calculation of the Stark Effect

Schrödinger's interest in applying the methods of undulatory mechanics to the problem of the Stark effect was awakened at a very early

stage of the whole enterprise. On p. 12 of the notebook "Eigenwertproblem des Atoms. I"—i.e., in the part that he composed during the first weeks of January 1926, perhaps even before returning from the Arosa Christmas vacation to Zurich—he included in a *Programm*, besides the problem of the action of a magnetic field on the atom, a second point, entitled "E-Feld. Parabelkoordinaten. v-Spektrum?" ("E-Field. Parabolic Coordinates. v-Spectrum?").

The key to solving the eigenvalue problem for the hydrogen atom in a homogeneous electric field of strength F in the z-direction, which is described by the wave equation

$$\Delta \psi + \frac{8\pi^2 m_e}{h^2} \left( E + \frac{e^2}{r} - eFz \right) \psi = 0 \tag{141}$$

—with  $m_e$ , e and h denoting the mass and charge of the electron and Planck's constant, respectively—consists of introducing—as Paul S. Epstein<sup>(328)</sup> had done a long time before—parabolic coordinates into the problem. Schrödinger selected spatial parabolic coordinates defined by the equations

and

$$x = +\sqrt{\lambda_1 \lambda_2} \cdot \cos \phi, \qquad y = +\sqrt{\lambda_1 \lambda_2} \cdot \sin \phi$$
$$z = \frac{1}{2}(\lambda_1 - \lambda_2) \tag{142}$$

which, for example, Hendrik Kramers had used in his doctoral dissertation. Kramers' equation for the action function S of the Stark effect problem, i.e., <sup>(329)</sup>

$$\frac{1}{\lambda_1 + \lambda_2} \left\{ \frac{1}{2m_e} \left[ 4\lambda_1 \left( \frac{\partial S}{\partial \lambda_1} \right)^2 + 4\lambda_2 \left( \frac{\partial S}{\partial \lambda_2} \right) + \frac{1}{\lambda_1} + \frac{1}{\lambda_2} \right) \left( \frac{\partial S}{\partial \phi} \right)^2 \right] - 2e^2 - \frac{1}{2}e(\lambda_1^2 - \lambda_2^2) F \right\} = E$$
(143)

might have offered Schrödinger an immediate opportunity to establish a wave equation on the lines suggested in his first communication. The same wave equation, however, followed in a more systematic manner from the principles laid down in the second communication, especially by transforming the fundamental wave equation, Eq (113), to parabolic coordinates. Thus one obtained the equation

$$\frac{\partial}{\partial\lambda_1} \left( \lambda_1 \frac{\partial\lambda}{\partial\lambda_1} \right) + \frac{\partial}{\partial\lambda_2} \left( \lambda_2 \frac{\partial\lambda}{\partial\lambda_2} \right) + \frac{1}{4} \left( \frac{1}{\lambda_1} + \frac{1}{\lambda_2} \right) \frac{\partial^2}{\partial\phi^2} + \frac{2\pi^2 m}{h^2} \left[ E(\lambda_1 + \lambda_2) + 2e^2 - \frac{1}{2}eF(\lambda_1^2 - \lambda_2^2) \right] \psi = 0$$
(144)

Evidently, Eq. (144) could be split into three second-order differential equations, each involving derivatives with respect to a single parabolic coordinate, namely,

$$\frac{\partial^2 \Phi}{\partial \phi^2} = -n^2 \phi \tag{144a}$$

and

$$\frac{\partial}{\partial\xi} \left(\xi \frac{\partial A}{\partial\xi}\right) + \left(D\xi^2 + A\xi + 2B + \frac{C}{\xi}\right)A = 0$$
 (144b, c)

where the full wave function is the triple product

$$\psi = \Phi(\phi) \cdot \Lambda_1(\lambda_1) \cdot \Lambda_2(\lambda_2) \tag{145}$$

Further,  $\xi$  and  $\Lambda$  stand for  $\lambda_1$  and  $\Lambda_1(\lambda_1)$  in Eq. (144b), while  $\xi$  and  $\Lambda$  stand for  $\lambda_2$  and  $\Lambda_2(\lambda_2)$  in Eq. (144c). The coefficients  $\Lambda$  and C are given by the expressions

$$A = \frac{2\pi m_e E}{h^2}$$
 and  $C = -\frac{n^2}{4}$  (146)

with *n* an integral constant (=0, 1, 2, 3,...); the coefficients *B* and *D* are given by

$$B_1 = \frac{\pi^2 m_e}{h^2} (e^2 - \beta)$$
 and  $D_1 = -\frac{\pi_2 m_e eF}{h^2}$  (147)

in the case of Eq. (144b) for  $\Delta_1(\lambda_1)$ , and

$$B_2 = \frac{\pi m_e}{h^2} (e^2 + \beta)$$
 and  $D_2 = + \frac{\pi m_e eF}{h^2}$  (148)

in the case of Eq. (144c) for  $\Lambda_2(\lambda_2)$ , with  $\beta$  a constant.

The solution of Eqs. (144) in the field-free case—i.e., in the absence of the Stark term  $D\xi^2$ —and for energy smaller than zero (A < 0, bound states), yielded the well-known Balmer term formula,

$$E = -\frac{2\pi^2 m_e e^4}{l^2 h^2}$$
(149)

with the integral "principal quantum number" l given by the equation

$$l = k_1 + k_2 + n + 1 \tag{150}$$

The quantities  $k_1$  and  $k_2$  have to assume, like *n*, integral values, i.e.,

$$n, k_1, k_2 = 0, 1, 2, 3, \dots$$
(150a)

because of the uniqueness conditions imposed on the functions  $\Phi$ ,  $\Lambda_1$ , and  $\Lambda_2$ . However, in the first-order perturbation approximation, the total energy of the hydrogen atom in the electric field became

$$E = -\frac{2\pi^2 m_e e^4}{l^2 h^2} - \frac{3}{8} \frac{h^2 Fl(k_2 - k_1)}{\pi^2 m_e e}$$
(151)

Schrödinger concluded: "It is the well-known formula of Epstein for the term values in the Stark effect of the hydrogen spectrum."<sup>(330)</sup> The integral numbers  $k_1$  and  $k_2$  corresponded to the "parabolic quantum numbers," which might also assume—like the integer n—the value zero. The analogue to the old "equatorial quantum number" in the new scheme was the number n + l, and Schrödinger noticed happily: "The value for the *latter* is thus automatically excluded by wave mechanics, just as by Heisenberg's mechanics."(331) Indeed, in the old quantum theory, electron orbits passing through the nucleus (as connected to the equatorial quantum number zero) had to be arbitrarily excluded, while in the quantum mechanics developed by Heisenberg the exclusion happened automatically. With the reproduction of this result, Schrödinger's Stark effect calculation could be considered as a complete success. In this paper, the third communication on "Quantization as an Eigenvalue Problem," Schrödinger also developed a detailed perturbation theory for many degress of freedom-which he applied to the theory of the Stark Effect.

# 14. RESPONSE TO WAVE MECHANICS. I. THE EARLY PHASE

After the submission of the first two communications on "Quantisierung als Eigenwertproblem," the close relations between Munich and Zurich continued. Of course, contact with Wilhelm Wien had to be kept up automatically, because Schrödinger went on to write and send further papers on wave mechanics to the editor of Annalen der Physik. As a rule, he requested that Wien show the manuscripts to Arnold Sommerfeld first. But this formal, official business was not all: besides giving certain explanations concerning the contents of the papers, Schrödinger reported other important events to Wien, especially the further successes of the new theory and its propagation.

On March 17, 1926, Schrödinger sent Wien the manuscript of the paper containing the demonstration of the equivalence of wave and matrix

mechanics; two days afterwards he commented on the results of the paper, upon which Wien replied promptly: "Your last essay I have sent immediately to the printing office, since Sommerfeld [to whom Schrödinger had requested that Wien show the paper beforehand ] is still in England."<sup>(332)</sup> Wien wrote further: "It is highly astonishing and delightful to observe how fast the steps proceed; your new result, which establishes the mathematical bridge to the matrix theory, certainly does not leave any doubt about the fact that you have chosen the right path."<sup>(331)</sup> Schrödinger, for his part, felt "extremely happy that men like you and *Geheimrat* Planck share the good hopes for the path I have chosen," because this positive attitude did not prevail in general.<sup>(333)</sup> He remarked: "It seems at present that the conviction does not exist everywhere that one should welcome without reservation a renunciation of the fundamental discontinuities, if one can do so."<sup>(333)</sup> He further added that he had "always ardently hoped that this would be possible" and that he "would have seized it with both hands"-as much as in the case of the Bohr-Kramer-Slater theory-"even if chance had not played the first (in view of de Broglie I should more correctly say second) tip directly into my own hands."(333) He again thanked Wien most heartily, in particular for his "strong advocacy in favor of the classical theory," and added the remark: "It would be nice if one were allowed again to think in a clear and simple way instead of in terms of verdicts and commandments, rules and correspondence-like analogies-which certainly constituted an unavoidable and highly appreciable intermediate situation."<sup>(333)</sup>

Sommerfeld, although he did not share Wien's antipathy towards the erstwhile [i.e., matrix mechanical] status of quantum theory, nevertheless followed Schrödinger's work with extreme interest. He spread the news about wave mechanics not only by letters, but also in his public talks and lectures such as those he delivered in England in March 1926.<sup>(334)</sup>

The exchange of scientific ideas on problems of statistical mechanics with Max Planck and Albert Einstein had contributed crucially in 1925 to Schrödinger's getting on to the path to wave mechanics. After he had submitted the paper on "*Die Energiestufen des idealen einatomigen Gasmodells*" ("The Energy Levels of the Ideal Monatomic Gas Model") at the beginning of December 1925,<sup>(213)</sup> the connection with Berlin was interrupted for a while, hence the people there heard about the establishment of the new atomic theory later than their colleagues in Munich. Still, they learned about wave mechanics earlier than other scientific circles, and they did so through personal reports by Schrödinger. As a result, they had the opportunity of responding to his ideas very early.

Writing to Planck, Schrödinger reported briefly "about a thing which has captured me completely for two months and which—I am already totally convinced about—possesses a quite extraordinary significance."<sup>(335)</sup> He then formulated the "thing" in the case of conservative systems of classical mechanics, since—as he wrote—the generalization to relativistic atomic systems and to systems in a magnetic field did not yet work. Schrödinger summarized the problems which he had solved so far: namely, the nonrelativistic hydrogen atom, the rigid rotator, the one-dimensional oscillator, the rotating and oscillating diatomic molecule, and the Stark effect of first order of the hydrogen lines. Since the results of the calculations seemed to be very encouraging, he continued optimistically:

I do have the very boldest hopes that one would now succeed in constructing a harmonious quantum theory, free of all roughness, not in the sense that everything becomes continuously more discontinuous and represented more by integral numbers, but rather in the opposite sense: the beautiful classical methods [of second-order differential equations with boundary conditions] provide automatically all the integralness that is necessary; this is no mysticism of integral numbers, *keine Mystik in den ganzen Zahlen*) but just the same integral numbers, which we are used to since long as occurring in surface harmonics, Hermitian and Laguerre polynomials (the former for the oscillator, the latter for the hydrogen electron).<sup>(335)</sup>

After this enthusiastic report, Schrödinger added a word of caution: "I do not, of course, mean that now one can again explain everything by ordinary mechanics, that the  $\psi$ -vibrations are mass vibrations in the sense of the usual mechanics. On the contrary: they or something similar seems to be at the basis of all mechanics and electrodynamics."<sup>(335)</sup> He concluded this highly informative letter with the words: "Please forgive me, highly revered Herr Geheimrat, the unsatisfactory aspect of this short presentation; I cannot report the things with much more clarity in a few pages."<sup>(335)</sup> Within a month, however, Schrödinger had available reprints of proof-sheets of his first two communications on "Quantisierung als Eigenwertproblem"<sup>(244,256)</sup>; he immediately dispatched copies to Max Planck in Berlin. This started an exchange of several letters on wave mechanics between Planck and Schrödinger during the period between April and June 1926.

Planck acknowledged the receipt of Schrödinger's paper in a postcard:

Many thanks for the reprint. I read your article the way an inquisitive child listens in suspense to the solution of a puzzle that he has been bothered about for a long time, and I am delighted with the beauties that are evident to the eye, but I have to study it much more closely and in detail to be able to grasp it completely. Besides, I find it extremely congenial that such a prominent role is played by the action function W. I have always been convinced that its significance in physics was still far from exhausted.<sup>(336)</sup>

Planck's extremely positive reception of wave mechanics also affected Albert Einstein, who wrote a letter to Schrödinger two weeks later. He started by saying: "Professor Planck pointed your theory out to me with well-justified enthusiasm and I studied it too, with the greatest interest."<sup>(337)</sup> Schrödinger immediately wrote to Einstein: "My sincere thanks for your extremely kind letter of the 16th. Your approval and Planck's mean more to me than that of half the world. Besides, the whole thing would certainly not have originated yet, and perhaps never would have (I mean, not from me), if I had not had the importance of de Broglie's ideas really brought home to me by your second paper on gas degeneracy."<sup>(338,339)</sup>

Einstein acknowledged Schrödinger's answer quickly. He wrote back: "I am convinced that you have made a decisive advance with your formulation of the quantum condition, just as I am equally convinced that the Heisenberg-Born route is off the track."<sup>(340)</sup> Two days after Einstein wrote the letter, Werner Heisenberg presented the Göttingen quantum mechanics at the Berlin *Kolloquium*, providing Einstein more detailed information about this theory. He faced a critical Einstein, who had already concerned himself with what he called the "Heisenberg-Born scheme" for some time.<sup>(341)</sup>

Schrödinger kept Einstein, Planck, and Hendrik Lorentz informed about the latest progress of wave mechanics by sending them reprints-or proof-sheets-of his papers. Lorentz, in particular, responded to Schrödinger on many points of detail.<sup>(342)</sup> Planck, on the other hand, expressed his pleasure that "we may soon have the opportunity to hear you and talk to you here."(343) Schrödinger had already been invited to Berlin sometime earlier to present a talk at a meeting of the German Physical Society. Planck had discussed with Eduard Grüneisen, then President of the Berlin Section, and now mentioned in his letter, the possibility of having Schrödinger's visit during the summer semester, i.e., before the end of July. Hence he wrote enthusiastically: "Let me tell you explicitly how much pleasure all of the physicists here would have in having you yourself present your new theory and coming into contact with your ideas."(343) After a further exhange of letters between Schrödinger and Planck, it was agreed that Schrödinger would give a talk at the Berlin Physical Society on July 16. This talk was expected to be on the level of "students in the upper classes who, therefore, have already had mechanics and geometrical optics, but who have not yet advanced into the higher realms; to whom, therefore, the Hamilton-Jacobi differential equation signifies ... not by any means something to be taken for granted"; hence Schrödinger should give "a general survey of the fundamentals for the purpose of orientation without much calculation and without many individual problems."(344) Planck went on to say: "Perhaps it would be easier and more natural for you to carry this out, if on the other day, Saturday morning the 17th of July, you were to give a second lecture in our Colloquium, aimed at more special matters

with supplements and continuations of the lines of thought you will have described at the more general meeting."  $(^{344})$ 

Planck also invited Schrödinger to stay at his house during the Berlin visit, as "my wife and I would be especially happy if you would stay with us," promising him to "have the opportunity to withdraw and occupy yourself as you see fit."<sup>(344)</sup> Schrödinger accepted the dates of the lectures as well as the invitation to Planck's home "with the utmost pleasure." He wrote back: "The words with which you offer me your house as a 'place of refuge from Berlin' express a boundless, thoughtful, concerned kindness that has truly touched me."<sup>(345)</sup> He hoped to be able, despite his end-ofsemester fatigue, to "give as much as I possibly can, both in and outside the 'official' hours, to the gentlemen in Berlin who are so friendly as to be interested in my work"; he would like, "from a purely selfish standpoint ... to make full and intensive use of the opportunity to discuss the things that have held me completely captured for months, with a number of the most distinguished scientists with the widest variety of research interests."<sup>(345)</sup> Schrödinger finally announced—after mentioning in his letter some recent results on an application of wave mechanics to dispersion theory-that he would like to arrive in Berlin on the evening of July 15, 1926.

In a letter dated June 15, Planck confirmed the arrangements of the lectures to the Physical Society (on July 16, 1926) and to the Berlin *Kolloquium* (on July 17, 1926). He wrote further: "On the evening of the 17th I hope to have several colleagues and you at our home," indicating that he planned to have a party at his house, where Schrödinger might meet and discuss more privately with some of the eminent Berlin physicists. As Planck had expected, Schrödinger's visit—including his talk on "*Grundlagen einer auf Wellenlehre begründeten Atomistik*" ("Foundation of an Atomic Theory based on the Wave Approach") before the Physical Society and the Colloquium lecture—was very successful. The acquaintance with Berlin and the physics community there would contribute to the invitation to Schrödinger, within less than a year, to take up the chair of theoretical physics at the University of Berlin as the successor of Max Planck.

# 15. FORMAL EQUIVALENCE OF WAVE MECHANICS AND THE QUANTUM MECHANICS OF BORN, HEISENBERG, JORDAN, AND DIRAC

On seeing the manuscript of Schrödinger's first communication on *Quantisierung als Eigenwertproblem*, Arnold Sommerfeld wrote to Schrödinger: "My first impression is this. Your method is a substitute for

the new quantum mechanics of Heisenberg, Born, and Dirac (*Proc. R. Soc.* London, 1925), in particular a simplified one—so-to-say, an analytical resolvent of the algebraic problem posed there [i.e., in quantum mechanics]."<sup>(275)</sup> Sommerfeld was deeply impressed by the new, so completely different atomic theory, and he immediately thought of connecting it to the quantum mechanical scheme developed earlier. Obviously, he mentioned this to his experimental colleague Wilhelm Wien, who soon emphasized the same point in his own letter to Schrödinger. Wien reported: "Sommerfeld thinks that your theory agrees with that of Heisenberg and Born. Since I do not know the latter, I cannot judge it."<sup>(274)</sup>

In a letter, dated March 4, 1926, Schrödinger asked Wien to include some corrections to his second communication on *Quantisierung als Eigenwertproblem*, but did not report any news on the problem of relating the two theories. However, two weeks later a radical change occurred: on March 18 Wien received a completely finished and polished article from Schrödinger, entitled "*Über das Verhältnis der Heisenberg-Born-Jordanschen Quantenmechanik zu der meinen*" ("On the Relation between the Heisenberg-Born-Jordan Quantum Mechanics and My Own"), which was intended to be published in the *Annalen der Physik*. Schrödinger wrote to Wien:

The hope which I expressed in point 4 of my letter of February 22 has been fulfilled much earlier than I thought. The relationship [of my theory] to Heisenberg's has now been completely clarified, and this in the sense that anyone who does not want also must not calculate with matrices, since both representations are—from the purely mathematical point of view—totally equivalent. From the physical point of view, though, my representation seems to me to be considerably more satisfactory and expandable (*ausbaufähiger*), because one is guided by intuition. Also, the fact that I succeeded from the point of view of undulatory mechanics in revealing the relation [to Heisenberg's theory], while Weyl—with whose mathematical knowledge and ability I cannot [even] remotely compare—did not manage it from the matrix point of view, speaks a *posteriori* in favor of the superiority of my theory and of the much better prospect it also provides as far as the mathematical methods are concerned.<sup>(346)</sup>

Wien reacted to Schrödinger's announcement with enthusiasm, and wrote back: "Your new result, which at least provides the mathematical bridge to the matrix theory, certainly no longer leaves any doubt that you are proceeding on the right path."<sup>(349)</sup>

Schrödinger outlined his view on the problem of establishing a relationship with what he abbreviated as "Heisenberg's quantum mechanics" (meaning the matrix theory of Born, Heisenberg, and Jordan) in the introduction of the new paper as follows:

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,  $^{(244,256)}$  it is very strange that these two new theories agree with one another with regard to the known facts even where they differ from the old quantum theory.... That is really very remarkable, because starting points, presentations, methods, and in fact the whole mathematical apparatus, seem fundamentally different. Above all, however, the departure from classical mechanics in the two theories seems to occur in diametrically opposite directions. In Heisenberg's work the classical continuous variables are replaced by systems of discrete numerical quantities (matrices) which depend on a pair of integral indices, and are defined by *algebraic* equations. The authors themselves [i.e., Born, Heisenberg, and Jordan (1926, p. 79)]<sup>(348)</sup> describe the theory as a "true theory of a discontinuum." On the other hand, wave mechanics shows just the reverse tendency; it is a step from the classical point-mechanics towards a *continuum theory*.<sup>(349)</sup>

Indeed, one could hardly imagine a bigger antagonism than that existing between the undulatory mechanics, in which a "continuous *fieldlike* process in configuration space ... governed by a single *partial* differential equation" replaces the finite number of differential equations plus the quantum conditions describing a system of finitely many variables in the "classical quantum theory," on the one hand, and, on the other hand, the Göttingen approach which "connects the solution of a problem in quantum mechanics with the solution of a system of an infinite number of algebraic equations, in which the unknowns—infinite matrices—are allied to the classical position- and momentum-coordinates of the mechanical system, and functions of these, and obey peculiar *calculating rules.*"<sup>(350)</sup>

In order to establish a relation between the two schemes, Schrödinger planned to proceed in two steps. First, he showed how

to each function of the position- and momentum-coordinates there may be related a matrix in such a manner, that these matrices, *in every case, satisfy* the formal calculating rule of Born and Heisenberg. [He emphasized:] This relation of matrices to functions is *general*; it takes no account of the *special* mechanical system considered, but is the same for all mechanical systems.... However, the relation is still *indefinite* to a great extent. It arises, namely, from the *auxiliary introduction* of an *arbitrary* complete orthogonal system of functions having for domain *entire configuration space* [i.e., the full *q*-space].<sup>(351)</sup>

### As a second step, Schrödinger showed:

The special system of algebraic equations, which, in a *special* case, connects the *matrices* of the position and momentum coordinates with the *matrix* Hamilton function, and which the authors [i.e., Born, Heisenberg, and Jordan] call "equations of motion," will be completely solved by assigning the auxiliary role to a *definite* orthogonal system, namely, to the system of *eigenfunctions* of that partial differential equation which forms the basis of my wave mechanics. The solution of the natural *boundary-value problem* of this differential equation is *completely equivalent* to the solution of Heisenberg's algebraic problem.<sup>(352)</sup>

The entire demonstration thus resulted, as Schrödinger pointed out, in the conclusion:

From the formal mathematical standpoint, one might well speak of the identity of the two theories.... [Especially,] all Heisenberg's matrix elements, which may interest us from the surmise that they define "transition probabilities" or "line intensities," can be actually evaluated by *differentiation and quadrature*, as soon as the *boundary-value problem* is solved. [Wave mechanics even had, so Schrödinger claimed, the advantage of providing] these matrix elements, or quantities that are closely related to them ... the perfectly clear significance of amplitudes of the partial oscillations of the atom's electric moment, [thus making] the intensity and polarization of the emitted light intelligible on the basis of the Maxwell-Lorentz theory.<sup>(353)</sup>

## 15.1. Operators and Equivalence of Wave and Matrix Equations

Schrödinger showed, as a first step, that the Born-Heisenberg-Jordan scheme could be represented by an operator calculus; as a second step, he then proved the one-to-one relation between these operator methods and the wave mechanical equations and operations.

In his paper, Schrödinger wrote:

The crucial point in the construction of matrices is given by the simple observation that Heisenberg's peculiar calculating laws for functions of the *double* set of *n* quantities,  $q_1, q_2, ..., q_n$ ;  $p_1, p_2, ..., p_n$  (position- and canonically conjugate momentum-coordinates) agree exactly with the rules, which *ordinary* analysis makes *linear differential operators* obey in the domain of the *single* set of *n* variables,  $q_1, q_2, ..., q_n$ . So the coordination has to occur in such a manner that each  $p_1$  in the function is replaced by the operator  $\partial/\partial q_1$ . Actually the operator  $\partial/\partial q_1$  is *exchangeable* with  $\partial/\partial q_m$ , where *m* is arbitrary, but with  $q_m$  only, if  $m \neq 1$ . The operator, obtained by interchange and subtraction when m = 1, viz.

$$\frac{\partial}{\partial q_1} q_1 - q_1 \frac{\partial}{\partial q_1}$$
 [(152)]

when applied to any arbitrary function of the q's, reproduces the function, i.e., this operator gives *identity*. This simple fact will be reflected in the domain of matrices as Heisenberg's commutation rule.<sup>(354)</sup>

The above-mentioned starting point of Schrödinger's demonstration reminds one of the corresponding starting point of Max Born's translation—in July 1925—of Heisenberg's new quantization rule into the matrix language. At that time the replacement of Heisenberg's equation,<sup>(355)</sup>

$$h = 2\pi m \sum_{\tau = -\infty}^{+\infty} \left[ |q(n+\tau, n)|^2 \,\omega(n+\tau, n) - |q(n, n-\tau)|^2 \,\omega(n, n-\tau) \right] \quad (153)$$

by the equation (of Born)

$$\sum_{k} [p(n, k) q(k, n) - q(n, k) p(k, n)] = \frac{h}{2\pi i}$$
(154)

had led to the matrix relation

$$pq - qp = \frac{h}{2\pi i} \, 1 \tag{155}$$

and thus to the whole matrix scheme of quantum mechanics. Schrödinger now observed that the replacement of the momentum variable p by essentially the operator

$$p = K \frac{\partial}{\partial q}, \qquad K = \frac{h}{2\pi i}$$
 (156)

a procedure that he had already followed in the first attempt to derive the hydrogen wave equation,<sup>(356)</sup> led to an automatic satisfaction of the Born-Heisenberg-Jordan quantum condition.

This important observation provided a strong stimulus to try an attempt at "a systematic construction" of a simple operator formalism that would replace the matrix scheme of the Göttingen physicists. In presenting this attempt, Schrödinger followed to some extent the detailed steps which had been taken earlier by Born and Jordan when building up matrix mechanics.

The first point which he noticed was the following: in constructing the operator corresponding to a function of the position and momentum variables,  $q_k$  and  $p_k$ , one must take the commutation rule (155) and, therefore, prescribe a "function-symbol written in a definite way," which he called a "well-arranged" or "well-ordered function symbol."<sup>(357)</sup> For example, Schrödinger associated with a function of the type,

$$F(q_k, p_k) = f(q_1, ..., q_n) p_r p_s p_t g(q_1, ..., q_n) p_{r'} h(q_1, ..., q_n) p_{r''} p_{s''} \cdots$$
(157)

the well-ordered function-symbol

$$[F, \cdot] = f(q_1, ..., q_n) K^3 \frac{\partial^3}{\partial q_r \partial q_s \partial q_t} g(q_1, ..., q_n)$$
  
 
$$\cdot K \frac{\partial}{\partial q_{r'}} h(q_1, ..., q_n) K^2 \frac{\partial^2}{\partial q_{r''} \partial q_{s''}} \cdots$$
(158)

The operator  $[F, \cdot]$  may be applied to any function u of the position variables alone, and the same can be done with a product operator

 $[GF, \cdot]$ —which is defined such that first F is applied to u, and then G to the resulting function. Because of the commutation rule, Schrödinger observed in general that

$$[GF, \cdot] \neq [FG, \cdot] \tag{159}$$

With the "well-ordered function-symbol" following the same relations as the corresponding matrix symbol, Schrödinger proceeded to establish detailed operator expressions for the important matrix expressions of quantum mechanics. For that purpose he assumed that his operators acted on a complete orthogonal function system defined in the entire x-space (where x denotes the n coordinates  $q_1, ..., q_n$ ),

$$u_1(x)\sqrt{\rho(x)}, \quad u_2(x)\sqrt{\rho(x)}, \quad u_3(x)\sqrt{\rho(x)},...$$
 (160)

with each function  $u_i(x)$  vanishing fast enough at infinite x. He then associated with the operator (157) the matrix coefficients  $F^{kl}$  by the relation

$$F^{kl} = \int \rho(x) \, u_k(x) [F, u_l(x)] \, dx \tag{161}$$

which he verbally expressed as: "A matrix element is computed by *multiplying* the function of the orthogonal system [(160)] denoted by the row-index (whereby we always understand  $u_i$ , not  $u_i \sqrt{\rho}$ ) by the "density function"  $\rho$ , and by the result arising from using our operator on the orthogonal function corresponding to the *column*-index, and then by integrating the whole over the domain."<sup>(358)</sup> Schrödinger now went ahead and demonstrated explicitly how his "matrices"  $F^{kl}$  indeed obeyed the matrix relations of Born, Heisenberg, and Jordan.

First of all, the definition contained in Eq. (161) obeyed the rule of matrix multiplication, i.e.,

$$(FG)^{km} = \sum_{l} F^{kl} G^{lm}$$
(162)

Similarly, Schrödinger established the matrix mechanical rules for he (partial) differentiation of a (matrix) variable with respect to the position or momentum variable, namely,

$$\left[\frac{\partial F}{\partial q_1},\cdot\right] = \frac{1}{K} \left[p_1 F - F p_1,\cdot\right]$$
(162a)

$$\left[\frac{\partial F}{\partial p_1}, \cdot\right] = \frac{1}{K} \left[Fq_1 - q_1F, \cdot\right]$$
(162b)

or

The crucial point in the entire demonstration of equivalence between the matrix and the wave mechanics now had to do with the solution of the equations of motion. In matrix from the latter read

$$\left(\frac{\partial q_1}{\partial t}\right)^{ik} = \left(\frac{\partial H}{\partial p_1}\right)^{ik} \tag{163a}$$

and

$$\left(\frac{dp_1}{dt}\right)^{ik} = -\left(\frac{\partial H}{\partial q_1}\right)^{ik} \tag{163b}$$

with a suitably symmetrized Hamiltonian diagonal matrix  $(H^{ik})$ . Since the time derivative of the matrix element  $q^{ik}$  reproduced the matrix element multiplied by the factor  $2\pi i(v_i - v_k)$ , Eqs. (163) assumed the form

$$(v_i - v_k) q_1^{ik} = \frac{1}{h} (Hq_1 - q_1 H)$$
(164a)

and

$$(v_i - v_k) p_1^{ik} = \frac{1}{h} (Hp_1 - p_1 H)$$
 (164b)

Schrödinger made two essential claims:

1. The Eqs. [(164)] will in general be satisfied if we choose as the orthogonal system the eigenfunctions of the natural boundary value problem of the following partial differential equation:

$$-[H, \psi] + E\psi = 0$$
 [(165)]

 $\psi$  is the unknown function of  $q_1, q_2, ..., q_n$ ; E is the eigenvalue parameter.... The quantities  $v_i$  are found to be equal to the eigenvalues  $E_i$  divided by h.  $(H^{kl})$  becomes a diagonal matrix, with  $H^{kk} = E_k$ .

2. If the symmetricalizing of the function H has been effected in a suitable way—the process of symmetricalizing, in my opinion, has not hitherto been defined uniquely—then [Eq. (165)] is identical with the wave equation which is the basis of my wave mechanics.<sup>(359)</sup>

The use of the eigenfunctions of the differential equation (165) as the complete system  $u_i(x)$  for the operator formalism obviously led to the following matrix elements  $H^{kl}$ ,

$$H^{kl} = E_1 \int p(x) \, u_k(x) \, u_1(x) \, dx = \begin{cases} E_1 & \text{for } l = k, \\ 0 & \text{for } l \neq k \end{cases}$$
(166)

If inserted into the right-hand side of Eq. (164a), one obtains  $((E_i - E_k)/h) q_1^{ik}$ ; consequently, the transition frequency indeed assumes the value  $(E_i - E_k)/h$ , as has been asserted by Claim 1.

In order to prove the remaining, most important, Claim 2, Schrödinger recalled the derivation of his wave equation from the classical problem described by the Hamiltonian H,

$$H = \mathfrak{J}(q_k, p_k) + V(q_k) \tag{167}$$

where the kinetic energy  $\Im$  is supposed to be a quadratic form of the momentum variables  $p_k$  and the potential V depends only on the position variables  $q_k$ . In his first communication, he had proceeded by calling upon the variational principle

$$0 = \delta J_1 = \delta \int \left\{ \frac{h^2}{4\pi^2} \Im\left(q_k, \frac{\partial \psi}{\partial q_k}\right) + \psi^2 V(q_k) \right\} \Delta_p^{-1/2} dx$$
(168)

supplemented by the subsidiary condition

$$J_2 = \int \psi^2 \Delta_p^{-1/2} \, dx = 1 \tag{168a}$$

 $(\Delta p \text{ denoted the discriminant of the quadratic form } \mathfrak{J}.)$  When he carried out the variation in the following way,

$$0 = \frac{1}{2} (\delta J_1 - E \delta J_2) = \int \left[ -\frac{h^2}{8\pi^2} \sum_k \frac{\partial}{\partial q_k} \left( \Delta_p^{-1/2} \frac{\partial \mathfrak{J}}{\partial p_k} \right) + (V - E) \Delta_p^{-1/2} \psi \right] \delta \psi \, dx \tag{169}$$

the Eulerian equation

$$\frac{h^2}{8\pi^2} \Delta_p^{1/2} \sum_k \frac{\partial}{\partial q_k} \left( \Delta_p^{-1/2} \frac{\partial \mathfrak{J}}{\partial p_k} \right) - V \psi + E \psi = 0$$
(170)

followed immediately. By referring to the relation

$$\mathfrak{J}(q_k, p_k) = \frac{1}{2} \sum_k p_k \frac{\partial \mathfrak{J}(q_k, p_k)}{\partial p_k}$$
(171)

which is valid for quadratic form in the  $p_k$ , and by observing the relation (156), this equation transformed into Eq. (165). Schrödinger concluded triumphantly: "Hence the solution of the whole system of matrix equations of Heisenberg, Born, and Jordan is reduced to the natural

boundary-value problem of a linear partial differential equation. If we have solved the boundary value problem, then by the use of Eq. [(161)] we can calculate by differentiations and quadratures every matrix element we are interested in."<sup>(360)</sup>

Although he had confined himself to a nonrelativistic problem in atomic physics in which no external magnetic field occurred, he scarcely doubted "that the complete parallel between the two new quantum theories will stand when this generalization is obtained."  $(^{361})$ 

Schrödinger wrote to Sommerfeld on April 18, 1926: "With Pauli I have exchanged a couple of letters. He really is a phenomenal person. How he has discovered everything again? In a tenth of the time which I needed for it!" He evidently referred with these words to the recent news that he had received from Wolfgang Pauli, especially to what the latter called a "complete clarification of the connection of Schrödinger's theory and quantum mechanics" ("die Verbindung von Schrödinger mit der Quantenmechanik vollständig klargestellt").<sup>(362)</sup> Pauli obtained this clarification during a visit in the spring of 1926 to Copenhagen, where he had gone to discuss the burning problems of atomic physics in those days. On April 12, 1926. Pauli formulated the result of his considerations in a detailed letter addressed to Pascual Jordan in Göttingen. He wrote: "Today I want to write neither about my Handbuch article nor about multiple quanta. I will rather tell you the results of some considerations of mine connected with Schrödinger's paper "Quantisierung als Eigenwertproblem," which just appeared in the Annalen der Physik. I feel that this paper is to be counted among the most important recent publications. Please read it carefully and with devotion."(363) He further wrote to Jordan: "I think I now have completely clarified [the connection between the Born-Heisenberg-Jordan theory and the Schrödinger theory]. I have found that the energy values resulting from Schrödinger's approach are always the same as those of the Göttingen mechanics, and that from Schrödinger's functions  $\psi$ , which describe the eigenvibrations, one can in a quite simple and general way construct matrices satisfying the equations of the Göttingen mechanics. Thus at the same time a rather deep connection between the Göttingen mechanics and the Einstein-de Broglie radiation field is established."<sup>(363)</sup>

In his letter to Jordan, Pauli went to establish the full mathematical equivalence between the Born-Heisenberg-Jordan quantum mechanics and Schrödinger's wave mechanics. He concluded: "The problem of the asymptotic linkage [of the new theory] with the usual pictures in space and time for the limiting case of large quantum numbers remains unsolved. Yet it is a definite progress to be able to see the problems [of atomic theory] from two different sides [i.e., from matrix mechanics and wave mechanics]. It seems that one also sees now, how from the point of view of quantum mechanics the contradistinction between 'point' and 'set of waves' fades away in favor of something more general."<sup>(363)</sup>

At the end of May 1926, Carl Eckart from Pasadena, California, contributed a paper to the Proceedings of the National Academy of Sciences, in which he tried "to show, in a purely formal way, that the Schrödinger equation must be the basis for the Born, Jordan, and Heisenberg matrix calculus."<sup>(364)</sup> On June 7, 1926. Eckart completed a second paper and submitted it to Physical Reviews, where it was published in the issue of October 1926.<sup>(365)</sup> In it Eckart wrote: "The more recent advances in quantum dynamics made by Heisenberg, Born and Jordan, Dirac, and most recently, by Schrödinger, have led to various mathematical formulations of the various physical hypotheses involved. In the present paper it is proposed to give a unified mathematical treatment, which, though it cannot pretend to be the final form of the theory, leads to methods of solution of the equations of Born and Jordan, and Dirac, which are much simpler than those previously developed....The final achievement will be the inclusion of the results of Schrödinger in a single calculus with those of the other authors mentioned above. This would seem to be the strongest support which either of the two dissimilar theories have thus far received."(366) The essential point consisted, as Eckart argued, in the task of establishing a general method of calculating matrix elements (i.e., the matrix elements of the Born-Jordan theory) and of relating Schrödinger's method directly to the other quantum mechanical methods. For this purpose, Eckart developed a formal calculus which "includes the Born and Jordan matrix dynamics, and also the remarkable quantum condition of Schrödinger."<sup>(366)</sup> As an appropriate formal calculus to accomplish all that, he made use of the operator calculus, i.e., a slight generalization of methods that were available in the mathematical literature for some time, and furnished the proof of the formal equivalence of the theories of quantum mechanics and wave mechanics.

# 16. RESPONSE TO WAVE MECHANICS II. APPLICATIONS AND EXTENSIONS

Several eminent physicists—including Wien, Sommerfeld, Planck, Einstein, and Lorentz—reacted very quickly to the proposal of an undulatory theory of atoms, sometimes even before the publication of Schrödinger's first communication on the subject. However, these, in general very positive, responses from Munich, Berlin, or Leyden did not immediately result in active work by others. One noticed and applauded the concepts and results of wave mechanics; one criticized this or that assumption in it; still, neither Sommerfeld, Einstein, nor Planck personally

sat down to try out a new example not previously considered by Schrödinger, or suggested a further application or extension of the scheme. But all three spread the message of undulatory mechanics among their colleagues.

Schrödinger's publications on wave mechanics in Annalen der Physik stimulated considerable interest among the quantum physicists in Germany, Central Europe, and Scandinavia. For example, in Vienna, Ludwig Flamm, a former colleague and friend of Schrödinger, wrote a review of the principles of that theory for the Physikalische Zeitschrift, propably constituting the first review of the subject.<sup>(367)</sup> Erwin Fues. Gregor Wentzel, Ivar Waller, Max Born, Werner Heisenberg, and Paul Dirac, all at different universities in Europe, wrote substantial papers in which they applied undulatory mechanics to new problems and extended its scope. The Belgian Charles Manneback, then in Zurich, Fritz Reiche in Breslau, Walter Gordon in Berlin, and again Gregor Wentzel in Leipzig, the Russian Waldemar Alexandrow, then in Zurich, and the Dane Øyvind Burrau in Copenhagen, all made further applications of wave mechanics to atomic problems; foreign visitors and students in Germany, such as the American J. Robert Oppenheimer in Göttingen, also contributed their share to the application and extension of wave mechanics.

In America, the California Institute of Technology became a center for the early use of wave mechanics; there, Carl Eckart and Paul Sophus Epstein dealt with atomic problems in the framework of the undulatory theory. Several months later the physicists on the East Coast joined the bandwagon, when Ralph Kronig and Isidor Rabi worked out the symmetrical top in Schrödinger's scheme.

Remarkably little happened in France, the homeland of matter waves. The best-known contribution came from the Belgian physicists Théophile De Donder and Frans Henri van den Dungen from Brussels; in two notes, submitted to the Paris Academy of Sciences, they suggested a relativistic extension of Schrödinger's wave equation (which Schrödinger also proposed), arriving at similar results as several other colleagues-in Germany (Walter Gordon), Sweden (Oskar Klein), Russia (Vladimir Fock), and Hungary (Janos Kudar)-at that time. Louis de Broglie, the inventor of the conception of matter waves, did of course take notice of Schrödinger's work; in a note, also submitted to the Paris Academy of Sciences, he declared it as having "confirmed our ideas on the wave nature of mechanics" ("confirmé nos idées sur la nature ondulatoire de la mécanique").<sup>(368)</sup> Basically, he did not pick up on the new theory, because his own ideas deviated strongly from Schrödinger's; in particular, de Broglie stressed the particle aspect as representing the real nature of microscopic objects, rather than the undulatory aspect.

England was another country in which not much happened in Schrödinger's theory in 1926—apart from Paul Dirac's important work communicated in August of that year to the *Proceedings of the Royal Society of London*.<sup>(369)</sup> However, in early 1927 the situation changed completely when Charles Galton Darwin in Edinburgh became interested in a relativistic extension of the wave equation for atoms including electron spin.<sup>(370)</sup> British interest increased tremendously soon after the experimental verification of the existence of matter waves in the spring of 1927, in which George Paget Thomson and Alexander Reid from Aberdeen took an essential part.

## 16.1. Band Spectra in Undulatory Mechanics

On April 27, 1926, the Annalen der Physik received a paper on "Das Eigenschwingungsspektrum zweiatomiger Moleküle in der Undulationsmechanik" ("The Eigenvalue Spectrum of Diatomic Molecules in Undulatory Mechanics"), the author being Erwin Fues from Zurich. This paper constituted the first contribution to wave mechanics that did not come from Schrödinger himself.

The study of band spectra had always provided an excellent testing ground for new ideas in atomic theory. With the Bohr-Sommerfeld Schwarzschild,<sup>(372)</sup> approach Karl Torsten to atomic structure, Heurlinger,<sup>(373)</sup> Wilhelm Lenz,<sup>(374)</sup> and Adolf Kratzer<sup>(375)</sup> had developed an understanding of the line patterns in molecular spectra. In July 1925, Werner Heisenberg had treated various properties of band spectra from the point of view of the just-proposed new quantum mechanics. In February 1926, then, Schrödinger had laid, in Section 3 of his second communication, the foundation of the theory of band spectra in wave mechanics by discussing the "rigid rotator with free axis" (Section 3.2) and the "nonrigid rotator" (Section 3.3). The latter could be used, as Schrödinger remarked, to calculate the energy states of diatomic molecules. He had finally arrived at the formula

$$E = E_i + \frac{n(n+1)h^2}{8\pi^2 A} \left(1 - \frac{\varepsilon}{1+3\varepsilon}\right) + \frac{2l+1}{2}hv_0\sqrt{1-3\varepsilon}$$
(172)

with n and l corresponding to the rotational and oscillational quantum numbers in the old quantum theory, respectively,

$$n = 0, 1, 2, 3, ..., l = 0, 1, 2, 3, ...$$
 (172a)

and  $\varepsilon$  representing the small quantity

$$\varepsilon = \frac{n(n+1)h^2}{16\pi^4 v_0^2 A^2}$$
(172b)

where A denoted the moment of inertia of the molecule.

Equation (172) described the situation roughly. But Schrödinger also realized:

The  $\varepsilon$ -corrections in [Eq. (172)] do not yet take account of the deviations of the nuclear vibrations from the pure harmonic type. Thus a comparison with Kratzer's formula and with experience is impossible.<sup>(377)</sup> I only desired to mention the case provisionally.... The rotation-vibration problem of the diatomic molecule will have to be reattacked presently, the nonharmonic terms in the energy of the binding being taken into account. The method selected skillfully by Kratzer for the classical mechanical treatment is also suitable for undulatory mechanics. If, however, we are going to push the calculation as far as is necessary for the fineness of band structure, then we must make use of the theory of perturbation of eigenvalues and eigenfunctions.<sup>(378)</sup>

At the time when he made this statement, namely in late February 1926, Schrödinger already possessed the perturbation theory mentioned earlier, although he would publish the details of the scheme only later, in his third communication, together with an application to the Stark effect of hydrogen Balmer lines.<sup>(379)</sup>

Instead of carrying out the necessary refined calculation of the molecular eigenvalues himself, Schrödinger left the problem as an exercise to Erwin Fues, his assistant in Zurich. The latter indeed succeeded in performing the rather tricky evaluation skillfully, translating Kratzer's old approach into the undulatory mechanics.

Fues' work on the diatomic molecule clearly showed that he was able to master fully the methods of undulatory mechanics at this early stage, such that the could apply them to a very complicated case. His solution compared favorably with a result which Lucy Mensing in Göttingen had calculated a month earlier on the basis of matrix mechanics.<sup>(380)</sup>

# 16.2. Intensity Calculations of Schrödinger, Pauli, Wentzel, and Fues

The first intensity calculation for atomic lines in the new quantum mechanics was performed by Werner Heisenberg in his pioneering paper of July 1925: he succeeded in obtaining the transition amplitudes in the cases of the anharmonic oscillator and the (rigid) rotator—the latter satisfying the semiempirical intensity rules for multiplet spectra and anomalous Zeeman effects.<sup>(381)</sup> Max Born and Pascual Jordan had then proved Heisenberg's fundamental assumption "that the squares of the absolute values of the elements in a matrix representing the electrical moment of an

atom provide a measure of the transition probabilities."<sup>(382)</sup> Again, within the matrix scheme, Lucy Mensing in her paper, which she submitted in March 1926 to Zeitschrift für Physik, found the expressions for the intensities of lines contained in the band spectra of diatomic molecules.<sup>(380)</sup> Such successes in Göttingen quantum mechanics in computing the intensities of spectral lines had led Schrödinger (in his second communication) to state: "The strength of Heisenberg's programme lies in the fact that it promises to give the *line intensities*, a question that we have not approached as yet. The strength of the present attempt [i.e., of wave mechanics] lies in the guiding physical point of view.... For me, personally, there is a special charm in the conception ... of the emitted frequencies as 'beats' which I believe will lead to an intuitive understanding of the intensity formulas."<sup>(383)</sup>

On the other hand, the "guiding physical point of view," namely the "intuitive" picture of the process of emitting spectral lines in the atom, did cause Schrödinger some problems. While the clarification was underway, Schrödinger completed his not showing the relation of wave mechanical and matrix mechanical schemes.<sup>(349)</sup> In the last section of that paper. subtitled "Ausblick auf ein klassisches Verständnis der Intensität und Polarisation der emittierten Strahlung" ("Prospect of a Classical Understanding of the Intensity and Polarization of the Emitted Radiation"), he approached the intensity question from what he called "the cardinal question of all atomic dynamics..., that of the *coupling* between the dynamic process in the atom and the electromagnetic field."<sup>(384)</sup> He then concluded, in particular, that the component of the electric dipole moment in the direction of the (Cartesian) coordinate  $q_1$  determined the intensity and polarization of atomic radiation (emitted in the transition from the state k to the state m). Schrödinger immediately used the result to calculate the intensities of the Stark components in the hydrogen spectrum. Thus, in the third paper of his series on "Quantisierung als Eigenwertproblem," submitted about four weeks after the paper on the equivalence proof, he presented the results on the Stark components for the four hydrogen lines  $H_{\alpha}$ ,  $H_{\beta}$ ,  $H_{\nu}$ , and  $H_{\delta}$  in four tables, each of which contained both the computed values and the experimental data for the components polarized parallel and transverse to the applied electric field.<sup>(385)</sup>

Wolfgang Pauli had tried, after the calculation of the nonrelativistic hydrogen states, to obtain in matrix formulas for the intensities of the hydrogen lines also.<sup>(386)</sup> In spite of initially being very optimistic, he did not really make sufficient progress until several months later, i.e., after discovering wave mechanics. Then he wrote, for example, in a letter to Gregor Wentzel:

The application to the hydrogen atom, for which Schrödinger already calculated the eigenfunctions, is very simple, in principle, though not always so in technical

procedure. In particular, one obtains for the intensities of the *series lines* expressions that are *rational* functions of the quantum numbers, since the associated eigenfunctions are of the form of the exponential function times a polynomial. At first there result, however, intricate-looking (though *finite*) double sums, which I have not yet succeeded in simplifying in the general case. I am, however, convinced that essential simplifications are possible, perhaps even closed expressions might follow.<sup>(387)</sup>

A few weeks later, Pauli informed Alfred Landé of his further progress: "Recently T have derived, based on the connection between Schrödinger ['s theory] and [the] Göttingen [theory], formulas for the absolute intensity of the Balmer lines. Ladenburg is supposed to test them by dispersion measurements. Since, however, Schrödinger is calculating similar things himself, I do not yet know where, how, and when I shall publish the results."<sup>(388)</sup> Finally, he again wrote to Wentzel: "Schrödinger will publish my formulas on the H-intensities, such as I wrote to you some time ago, in his third communication—according to my 'letter-publication method' of long standing."<sup>(389)</sup>

At that time, Wentzel showed enthusiasm in exploring wave mechanics in order to solve all kinds of problems of atomic theory. For example, he worked on the intensities of the hydrogen spectrum—the discrete as well as the continuous part—, but Pauli informed him: "The normalization of the eigenfunctions of the continuous spectrum has already been worked out by Fues, and he has also made extended calculations on the subject."<sup>(389)</sup> Hence, Wentzel did not pursue the problem any further, but turned to a different intensity problem and published the results in a letter to *Naturwissenschaften*.<sup>(390)</sup>

Wentzel got the idea of calculating the intensities of X-ray spectra from Schrödinger's previous work on the intensities of the Stark effect components. Wentzel started his note by saying: "Schrödinger has shown recently [Ref. 349] that one can construct the matrices of Heisenberg's quantum mechanics from the eigenfunctions of his mechanical wave equation by simple quadratures. Therefore one is for the first time in possession of a generally applicable method of calculating the intensities of spectral lines on the prescriptions of quantum mechanics."(391) Since Schrödinger had already solved the problem of the Stark effect intensities. in which—as we know—Wentzel was also interested, he used the method in a slightly modified problem, namely: "Instead like Schrödinger [in the case of the Stark effect (Schrödinger, Ref. 379)], choosing a homogeneous, external [electric] field, I have selected an internal central field as perturbation, and carried out the analogous calculation."<sup>(391)</sup> Thus he not only reproduced Schrödinger's intensity ratios for the hydrogen Balmer lines in the case of no perturbation; in the case of finite perturbation through a central field, he obtained "another splitting of the lines than that by

Schrödinger, namely the one corresponding to the series structure of the alkaline spectra and the X-ray spectra, respectively." (392) Wentzel hoped that the evaluation might provide a success similar to that of Schrödinger for the Stark effect of hydrogen, expecting particularly reliable results for the spectrum of the lithium atom and the K- and L-lines of the X-ray spectra.

Unfortunately, in the case of the lithium spectrum (having an especially close hydrogenlike structure) no intensity data were available on p-, d-, and f-terms, while in the X-ray spectra the existence of radiationless jumps could possibly spoil the comparison with the theoretical calculations. Still, Wentzel did refer to observations on the *L*-spectra of tungsten that had been published by Axel Jönsson from Uppsala in a recent issue of Zeitschrift für Physik.<sup>(393)</sup> He concluded in general a satisfactory agreement, if he compared the sum of the intensities of the two lines (for a Sommerfeld doublet) and the three lines (for so-called "composed doublets"), respectively.

At the end of his note, Wentzel mentioned briefly that Helmut Hönl's intensity formulas for anomalous multiplets plus the associated selection rules<sup>(394)</sup> would also follow from the properties of Schrödinger's eigenfunctions—essentially integral relations between surface harmonics. Further, he argued that the intensity rules for rotation-oscillation band spectra, such as had been obtained earlier by Ralph Fowler on correspondence principle arguments, <sup>(395)</sup> could be derived from wave mechanics as well, because the eigenfunctions of the rigid rotator with free axis were related to the spherical harmonics.<sup>(396)</sup> However, Erwin Fues would deal in greater detail with this problem in his second paper on the band spectra in wave mechanics.<sup>(397)</sup>

Fues approached the problem with great care. He departed from a relation proposed by Schrödinger in his fourth communication on "Quantisierung als Eigenwertproblem"<sup>(398)</sup>: namely, that the spatial density of electricity in an atom was given by the product of the wave function  $\psi$  with its complex conjugate  $\psi$ . Now  $\psi$  contained all eigenvibrations of the system under investigation and therefore had to be written as

$$\psi = \sum_{l} a_{l} u_{l} \exp\left[2\pi i \left(\frac{E_{l}}{h}t + \delta_{l}\right)\right]$$
(173)

with  $u_l$  denoting the (time-independent) eigenfunction,  $E_l$  the energy,  $\delta_l$  a phase connected with the *l*th eigenvalue, and  $a_l$  an amplitude factor—which depended, for example, on excitation conditions, temperature, and radiation damping. The (*jl*)-component of the electric moment in the *q*-direction had the form

$$M_q^{jl} = q_j a_l q^{jl} \tag{174}$$

and the entensity of the total radiation with frequency  $v_{jl}$  in the direction q became

$$J_{v_{jl}} \sim v_{jl}^4 a_j^2 a_l^2 (q^{jl})^2 \tag{175}$$

Thus the problem of calculating the intensity of the transition line  $v_{jl}$  consisted, up to a factor, of finding the matrix elements  $(q^{jl})^2$ , where q represented the various position variables of the system.

In the case of the x-, y-, and z-vibrations of band spectra, the "relative" intensities—especially up to the frequency factor—are

$$\frac{X}{Y}\Big|_{ln,l'n'} = \sum_{m=0}^{n} \sum_{m'=0}^{n'} \left\{ \int \left| \frac{x}{y} \right| u_{lnm} u_{l'n'm'} dt \right\}^{2}$$
(176)

Of course, the  $u_{lnm}$  were the eigenfunctions which he had calculated previously, and the *t*-integration extended over the entire three-dimensional space. In the case of the continuous spectrum he now derived the eigenfunctions

$$u_{nm}(E) = a_r \rho^{(k-1)/2} G_n(E, p) a_\theta P_{nm}(\cos \theta) \cdot a_\phi \begin{cases} \sin(m\phi) \\ \cos(m\phi) \end{cases}$$
(177)

where the radial eigenfunction  $G_n(E, \rho)$ —with E an eigenvalue in the continuum (i.e., for the two atoms of the molecule being separated—can be represented by exponential functions.<sup>(399)</sup>

The evaluation of Eqs. (176) for the discrete molecular spectrum provided the known selection rules: thus, for the x- and y-components only transitions with  $m - m' = \pm 1$ , and for the z-component only transitions with m = m', have finite intensities. All the nonzero components possess the same intensity, namely,

$$X \bigg|_{ln,l'n'} = r_0^2 \bigg(\frac{\kappa}{2}\bigg)^{dl} \frac{l!}{l'!} \frac{n}{3}, \quad \text{with} \quad \kappa = \frac{h}{4\pi^2 v_0 A^2}$$
(178)

After a lengthy calculation, Fues found—e.g., for transitions within the continuous spectrum of the diatomic molecule—a result that formally resembled the expression for transitions between discrete states, Eq. (178), that is,

$$J \sim r_0^2 \kappa^{3/2} \left(\frac{2}{e}\right)^{k'}$$
(179)

where k' assumes a value of about 200, and e denotes the base of natural logarithm. In spite of several questionable assumptions which he made

along the way, Fues concluded that his result, namely, the intensity [of the continuous spectrum] "starts with a nearly constant value right at the onset of the continuous spectrum, which therefore must possess a sharp edge,"<sup>(400)</sup> was correct at least in a qualitative sense.

# 16.3. Second-Order Stark Effect and the Hydrogen Spectrum

On July 16, 1926, Ivar Waller from Götteborg sent, in a letter to Erwin Schrödinger, a copy of a paper on the calculation of the secondorder Stark effect of hydrogen based on wave mechanics.<sup>(401)</sup> The first quantum mechanical calculation of the Stark effect had been performed by Wolfgang Pauli in the autumn of 1925 on the basis of the matrix theory, and had been included in Section 5 of his paper on the hydrogen spectrum.<sup>(386)</sup> Pauli only took into account the effect proportional to the strength of the electric field, obtaining the so-called Stark effect of first order in complete agreement with the old result of Paul Epstein on the basis of the Bohr-Sommerfeld theory.<sup>(328)</sup> When Waller began to work on the problem, he knew-from a remark at the end of Schrödinger's second communication<sup>(256)</sup>—that Schrödinger had meanwhile arrived at the same conclusion in wave mechanics. Waller therefore immediately turned to the more complicated problem of the *second-order* Stark effect within the wave theory, asking in particular whether the terms proportional to the square of the electric field strength also came out the same as in the old quantum theory. He obtained the energy corrections in the electric field F (with  $E = E_0 + E_1 F + E_2 F^2 + \cdots V$  as

$$E_1 = -\frac{3h^2}{8\pi^2 m_e eZ} nn_e \tag{180a}$$

and

$$E_2 = -\frac{h^6}{16(2\pi)^6 m_e^3 e^6 Z^4} n^4 (17n^2 - 3n_e^2 - 9k^2 + 19)$$
(180b)

with

$$-n+k+1 \leqslant n_e \leqslant n-k-1 \tag{180c}$$

where *n* and *k* are integral numbers, and *Ze* is the charge of the nucleus. On the second-order term  $E_2$ , Waller remarked: "This expression deviates formally from the one given by Epstein only by the fact that the term + 19 [in parentheses] has been added. One should note, however, that in the new quantum mechanics the value k = 0 is also admitted. Therefore, one obtains for small quantum numbers energy values that are totally different from Epstein's—for n = 1, e.g., the  $4\frac{1}{2}$ -fold value."<sup>(402)</sup>

Waller was not the only one to arrive at Eqs. (180) for the Stark effect. On the same day as he signed his paper, June 18, 1926, the *Zeitschrift für Physik* received a paper from Gregor Wentzel, in which he proposed an approximative solution method for Schrödinger's equations.<sup>(403)</sup> On applying it to the hydrogen atom in a constant external electric field F, Wentzel found the energy formula

$$E_{n_1 n_2 n_3} = -\frac{2\pi^2 m_e e^4}{h^2 n^2} - \frac{3h^2 F}{8\pi^2 m_e e} n(n_1 - n_2) - \frac{h^6 F^2}{2^{10} \pi^6 m_e^3 e^6} n^4 [17n^2 - e(n_1 - n_2)^2 - 8(n_3 - 1)^2 + 19]$$
(181)

When one puts Z=1 in Waller's formulas (180), and in addition  $n_e = n_1 - n_2$  and  $k = n_3 - 1$ , then the identity of the two results becomes evident. Both Waller and Wentzel compared their formula to the available data on the second-order Stark effect, and found good agreement.

Waller and Wentzel profitted in their contributions from the fortunate situation in that they learned of the recent work on atomic theory, in particular the papers of Heisenberg and Schrödinger, very early, often prior to publication. The physicists in America at that time did not share this advantage. Thus Carl Eckart in Pasadena only learned of Schrödinger's Annalen der Physik communications on wave mechanics after considerable delay (about a couple of months), which took away priority from his own work on the equivalence proof. Eckart also expressed doubts about the completeness of the description of the hydrogen atom in wave mechanics without involving the electron spin hypothesis<sup>(404)</sup>; he had no information about the discussions that were taking place on this subject thousands of miles away in Central Europe.<sup>(405)</sup> In July 1926, he knew that the problem of computing line intensities in the undulatory theory had meanwhile been solved for several atomic systems, such as the band spectra of diatomic molecules, the hydrogen spectrum and its Stark effect. Nevertheless, Eckart attacked the problem of computing the intensities of Balmer lines, but found that his results were not in agreement with observation. He noted, however: "The model is certainly incomplete, as is shown by the energy levels of the fine-structure predicted by this theory. The rotation [spin] of the electron ... is expected to remove this discrepancy."<sup>(406)</sup>

Whereas Eckart's results on the hydrogen line intensities appeared not to bear too much resemblance with observations, another wave mechanical calculation made in Pasadena, that of Paul Epstein on the Stark effect, certainly did. Epstein had (back in 1916, then at Munich) been responsible for the first successful interpretation of the Stark effect on the basis of the Bohr–Sommerfeld theory. Now, in the early summer of 1926, he was drawn—partly by his younger associate Carl Eckart—into the undulatory theory of atoms which, he soon realized, "opens new avenues of thought and seems to afford our first glimpse of the true nature of the quanta."<sup>(407)</sup> Epstein solved the differential equations for the Stark effect, obtaining eigenfunctions that could be expressed through hypergeometric functions. After a lengthy, but direct, evaluation he arrived at results for the energy terms which agreed in first order with the electric field strength with Waller's formula, Eq. (180a), if one replaces Waller's integral quantum number  $n_e$  by Epstein's (m-n). His expression for the second-order Stark effect, namely<sup>(408)</sup>

$$E_{2} = -\frac{D^{2}}{16Z^{4}m^{3}} \left(\frac{h}{2\pi e}\right)^{6} (m+n+s)^{4} \left[17(m+n+s)^{2} - 3(m-n)^{2} - 9s^{2} + 18s + 10\right]$$
(182)

becomes identical with Wallers's Eq. (180b) if one puts D = F and takes into account Epstein's different quantum numbers. In particular, there correspond:

Epstein: 
$$(m+n+s)$$
,  $(m-n)$ ,  $(s-1)$   
Waller:  $n$ ,  $n_e$ ,  $k$  (183)

Epstein further calculated the intensities of the Stark lines with the help of the Schrödinger-Eckart formulas for matrix elements. Epstein's intensity results did not fully coincide with those computed by Schrödinger. Epstein's calculation of the Stark effect intensities was not only independent of Schrödinger's,<sup>(398)</sup> but even yielded at times the more reliable result.

During the later months of 1926, another topic would arise in wave mechanics on which European and American physicists would work independently: the rotator and the symmetrical top. We shall report about this competition later.

# 16.4. Collision Processes in Wave Mechanics

On June 25, 1926, the Zeitschrift für Physik received a "preliminary communication" that was entitled "Zur Quantenmechanik der Stoßvorgänge" ("On the Quantum Mechanics of Collision Processes").<sup>(409)</sup> In the introduction to his note, Born explained the main goal of his communication: namely, to answer "the question about the very nature of [quantum-theoretical] 'transitions'."<sup>(410)</sup> He argued that (the Göttingen)

quantum mechanics constituted a logically complete theory which ought to describe the problem of atomic transitions properly. However, until now Born had not found a way of attacking the problem of transitions. Born also knew that in the collision problem continuous spectra of the particles involved in the interaction played a crucial role, hence the matrix formalism would not provide an easy access. Far more suitable appeared to be the operator methods, which he had developed at M.I.T. with the mathematician Norbert Wiener.<sup>(411)</sup> Since Schrödinger's theory could be considered as an extension of the Born-Wiener operator approach, and Born knew about the equivalence of matrix and wave mechanics (from Pauli's letter to Jordan in Göttingen, dated April 12, 1926), (363) he immediately turned to it, observing that it "alone proved to be [really] suitable in this case."<sup>(412)</sup> In his short note. Born discussed the introduction of a probability in the quantum mechanical collision problem; he argued, in particular, that it was necessary to give up the deterministic description of the scattering process. This conclusion became the starting point of a great debate that would be continued in the following decades. In a second paper on the quantum mechanics of collision processes, Born gave the details of the quantitative calculation; this paper was received four weeks later, on July 21, 1926, again by Zeitschrift für Physik.<sup>(413)</sup>

The fact that Schrödinger's wave mechanics allowed one to describe collision problems had induced Born to state in his first note: "I wish to consider it, just because of this reason, to be the deepest formulation of the quantum laws."<sup>(414)</sup> Happily he went on to work out, in early summer of 1926, the wave mechanical approach to general aperiodic atomic systems, i.e., situations in which the matrix mechanical description did not seem to be possible. The matrix formulation excluded the representation of atomic processes in space and time; in Schrödinger's theory, on the other hand, the atomic processes were actually described by wave motions which, of course, possess reality in space and time. Still, Born concluded: "Neither of these two interpretations seems satisfactory to me."<sup>(415)</sup> He suggested a third interpretation emerging from a remark of Einstein, namely that the wave field associated with radiation guides the corpuscular light-quantum like a "ghost field" ("Gespensterfeld"), i.e., it possesses no energy and momentum and determines the probability of a light-quantum (which is the carrier of energy and momentum) proceeding along a definite path. If Schrödinger's wave described the "ghost field" of mass particles, one had to conclude: "The guiding field, represented by a scalar function  $\psi$  of the coordinates of all particles involved and of time, propagates according to Schrödinger's differential equation. Momentum and energy, however, are transferred in such a manner as if corpuscles (electrons) do actually rush around. The orbits of these corpuscles are determined only insofar as they

are restricted by energy and momentum conservation; apart from this, only a probability for taking a definite path is determined by the value distribution of the  $\psi$ -function."<sup>(416)</sup> These statements involved a probability interpretation of the conventional orbit (a trajectory in space and time) of a particle; Born applied these ideas to extend the applications of quantum and wave mechanics to collision processes.<sup>(417)</sup> Born's wave mechanical collision theory seemed to be well in accord with the observed phenomena. This success also encouraged Born to derive conclusions, from his statistical interpretation of matter waves, on the nature of radiation phenomena. He asserted that "quantum mechanics … allows one to formulate and to solve the problem of transition processes," and that "Schrödinger's scheme seems in this situation to be by far the most suitable, adequate description."<sup>(418)</sup>

# 16.5. Cracking the Helium Problem

Heisenberg received the news about wave mechanics with some delay. He had left Göttingen at the end of the winter semester (in late February 1926) for an extended vacation; from there he first went to Munich (at the beginning of April) and had written to Pascual Jordan announcing that he would be back in Göttingen on April 20 and then go on to Copenhagen on April 24 or 25, where he was supposed to take up his position as lecturer in theoretical physics. On his way to Copenhagen, however, he had to make two stops: first, he went to Leipzig to discuss the offer of an extraordinary professorship at the University (April 25 to 26); then he presented (on April 28) a talk on quantum mechanics at the Berlin Kolloquíum. In Munich-at Sommerfeld's Institute-as in Göttingen and Berlin, he certainly heard more about Schrödinger's wave mechanics, but his many obligations did not leave him much time to take a deeper look at the new theory. Upon arriving in Copenhagen, he immediately assumed his duties as the successor of Hendrik Kramers, and simultaneously attacked a new task: the problem of calculating the helium spectrum in quantum mechanics.

The helium problem was an old acquaintance of Heisenberg's, and he had tried to develop a satisfactory theory of it since 1922. In this description, based of course on the old (Bohr–Sommerfeld) quantum theory of atomic structure, half-integral quantum numbers had played a crucial and controversial role. In the spring of 1926 such quantum numbers could be shown to arise at two different places in atomic theory: first, in the quantum mechanical formalism of angular momentum; and second, in the hypothesis of electron spin. The latter concept, especially, offered great hopes of providing a final, satisfactory solution of the helium problem. A
few days after his arrival (in late April 1926) in Copenhagen, Heisenberg wrote a postcard to Pauli in Hamburg stating that "we have found a rather decisive argument that your exclusion of equivalent orbits [of two electrons in an atom] is connected with the singlet-triplet separation," because: "Consider the energy written as a function of the transition probabilities. Then a large difference results, if one-at the energy of H atoms—has transition to 1S, or if, according to your ban [exclusion principle], one puts them equal to zero. That is, para- and ortho-[helium] do have independent energies, independently of the interaction between magnets [i.e., the magnetic moments associated with the spinning electrons]."<sup>(419)</sup> The new Copenhagen view seemed to be exactly along the lines on which Pauli expected to solve the helium problem, namely by a connection of his exclusion principle with the singlet-triplet separation. The idea now had to be carried out in a detailed quantum mechanical model. and this was what Heisenberg embarked on during the following three weeks. Then he rather happily reported to Born in Göttingen: "Since coming here I have worked very seriously on the helium spectrum, and I believe that now all the essential things are right; however, I have not yet completed the quantitative calculation."<sup>(420)</sup>

In his letter to Born, Heisenberg presented the main physical ideas of his solution to the helium problem, which was based on the assumption that the difference between corresponding ortho- and para-helium states arose from the Coulomb repulsion of the electrons. If, in particular, two electrons move around a (heavy) nucleus and the mutual influence of the electron spins was neglected, the (matrix) Hamiltonian of the system,  $H^0$ , consisted of the terms  $H^a$  and  $H^b$ , each referring to one electron moving under the influence of the Coulomb field of an effective nucleus (having a charge between e and 2e, due to the shielding of the other electron). Since the energy states  $H^a$  and  $H^b$  were exactly identical, the Hamiltonian  $H^0$ exhibited a particular degeneracy: the exchange of the two electrons in two different states, say  $W_n$  and  $W_m$ , would not alter the energy values of  $H^0$ . Only the Coulomb repulsion of the electrons removed the degeneracy; it could be treated in a matrix perturbation theory, yielding the first-order corrections

$$W_{nm}^{1\bullet} = H^1(nm, nm) + H^1(nm, mn)$$
(184a)

and

$$W_{nm}^{1\times} = H^1(nm, nm) - H^1(nm, mn)$$
 (184b)

Heisenberg commented on these results with the words: "For all following considerations the decisive result now is: The term system can be divided

into two separate parts (• and  $\times$ ), such that transitions occur only within the • system or within the  $\times$  system, but never from the • system to the  $\times$  system."<sup>(420)</sup>

Heisenberg assembled the details, which he had worked out, in a paper and submitted it two weeks later to Zeitschrift für Physik.<sup>(421)</sup> One of the major points proved in this paper was the fact that no transitions occurred between (•) and (×) terms. The reason was that the radiation amplitudes  $f_{n_1m_1,n_2m_2}$  of the unperturbed two-electron system were symmetric with respect to the exchange of the two electrons—i.e.,  $f_{n_1m_1,n_2m_2} = f_{m_1n_1,m_2n_2}$ —and the perturbed amplitudes obtained through a canonical transformation could be found to be

$$f'_{n_1m,n_2m} = f_{n_1m,n_2m} + f_{n_1m,m_2}$$
(185a)

for the transition between the dot-terms  $(n_1m) \rightarrow (n_2m)$  with  $n_1, n_2 < m$ , and

$$f'_{n_1m,mn_2} = f_{n_1m,n_2m} - f_{mn_1,mn_2}$$
(185b)

for the transitions between the dot- and cross-terms  $(n_1m) \rightarrow (mn_2)$  with  $n_1, n_2 < m$ . Evidently, the right-hand side of Eq. (185b) is zero and that of Eq. (185a) is finite. Finally, the singlet-triplet separation assumed the value

$$\Delta_{nm} = 2H(nm, mn) \tag{186}$$

where the perturbation matrix element  $H^1(nm, mn)$  would be physically interpreted as the difference of the perturbation energies created by the Coulomb repulsion between the electrons. The very same quantity should be responsible for the so-called Rydberg correction in the empirical term formula for the helium atom.

The above consideration could be extended to the case of the twoelectron atom containing real electrons with spin and associated magnetic moment. Again Heisenberg found that only transitions between dot- or cross-terms were possible (i.e., possessed finite amplitude). In this case each term system consisted of a singlet and a triplet system; the separation between similar terms of the singlet and the triplet, respectively, assumed—up to a small correction emerging from the magnet-magnet interaction—the value given by Eq. (186). Only one of the superterm systems, namely the one with triplet terms for ortho-helium and with singlet terms for para-helium, existed in nature.

At the time of writing his fundamental paper on the quantum mechanics of many-electron systems, Heisenberg also studied (in some detail) Schrödinger's first publications on wave mechanics. Indeed, he outlined at the end of Section 2 of his paper (dealing with the transition amplitudes between the term systems without electron spin) how to formulate the two-electron system in the language of undulatory theory. Thus the wave mechanical formulation offered a comfortable access to many-electron systems in quantum mechanics. Heisenberg said: "The great achievement of Schrödinger's theory is the calculation of matrix elements.... For the moment I want to go to Norway ... and to calculate there—besides mountaineering—quantitatively the helium spectrum. Why should one not once 'use the steamroller'?"<sup>(422)</sup> A few weeks after this vacation, the Zeitschrift für Physik received a second paper from Heisenberg on July 24, in which he presented his calculation of the helium and heliumlike spectra, i.e., the spectra of the series He, Li<sup>+</sup>, and Be<sup>++</sup>, etc.<sup>(423)</sup> Heisenberg obtained a general formula for the fine structure of two-electron spectra. In the special case of 2*p*-terms, where reliable data existed at that time, the formula

$$\Delta H_{2p} = \left(\frac{h}{2\pi}\right)^2 \frac{e^2}{2m_e^2 c^2} \left(\frac{\tilde{1}}{r^3}\right)_{2p} \left\{ (Z-3)(\frac{1}{2}, -\frac{1}{2}, -1) + (\frac{3}{8}, -\frac{3}{8}, \frac{3}{2}) - \frac{1}{4} \right\}$$
(187)

followed for the triplet separation (k = 1, j = 2, 1, 0). The pattern for the transition lines  $2p \rightarrow 2s$ , derived from Eq. (187), showed in the case of He two strong lines of narrow distance and a third faint line, and in the case of Li<sup>+</sup> three fairly separated lines, of which the third was much weaker. Qualitatively, this picture, especially the quasi-doublet structure of the ortho-helium lines, agreed with the then available data. Heisenberg was led to the following conclusion: "By the calculations carried out [in this paper] we wanted to show that quantum mechanics allows, even for atoms with two electrons, a quantitative description of the spectrum including finer details, and that the theory permits one to determine approximately the terms as a function of the quantum numbers." (424) At the same time, he pointed out the shortcomings of his approach, namely: (i) the lack of foundation in selecting the dot system (•), and (ii) the lack of accuracy in the calculations. Concerning the latter he added: "One should demand that the theoretical term values are computed so exactly that the agreement of these term values with the experimental values can be tested up to the last decimal."<sup>(424)</sup> In agreement with these statements, Heisenberg wrote to Pauli: "I have now submitted my paper on the helium spectrum, with dubious feelings, but [I am] not quite satisfied. All the calculations are too inaccurate and incomplete; the nicest thing is still the fine structure which comes out alright. In any case there remains, as far as quantitative agreement [with experiment] is concerned, much to be done."<sup>(425)</sup>

Heisenberg's dissatisfaction notwithstanding, his helium calculation

constitued a major triumph for quantum mechanics. It remained one of the standard approaches to two-electron problems which would be discussed in all later reviews of the topic; Heisenberg's successors would improve the approximation methods-so as to allow the treatment of the helium ground state or the excited S states—but the basic ideas did not have to be altered. In this respect, Heisenberg's helium calculation became a classic in atomic theory, and several decades later he recalled: "I used Schrödinger's formalism for help with the mathematics. It was clear to me that in order to calculate the shift of levels in the helium atom, matrix elements were needed, and they could be calculated quite well from Schrödinger's scheme. Such a calculation in matrix mechanics would have been difficult."<sup>(426)</sup> Thus the helium calculation-in spite of the fact that wave mechanical methods entered into it only as a tool for evaluating complicated matrix elements-also represented a major triumph of Schrödinger's theory, perhaps one of the greatest in view of the many unsuccessful efforts during the first half of the 1920s.

### 16.6. Symmetry Properties of Wave Functions and Quantum Statistics

Since Paul Dirac had developed a good quantum mechanical scheme of his own and was pursuing its consequences,<sup>(427)</sup> he was delayed in reading Schrödinger's first communication on wave mechanics. When he finally did study it, he was a trifle annoyed because he now had to learn about another method which obviously also worked well. In contrast to the people at Göttingen, however, whose first reaction was that Schrödinger's wave function could not have any real physical meaning, Dirac had no philosophical prejudice against it. Writing on "The Theory of Quantum Mechanics" in August 1926, Dirac referred to Schrödinger's work.<sup>(428)</sup>. He first mentioned the results which he had obtained earlier in attempting to solve the many-electron problem.<sup>(429)</sup> There the difficulty had arisen in finding a suitable set of "uniformizing" dynamical variables; it was connected the existence of an exchange phenomenon, noted for the first time by Heisenberg, arising from the fact that electrons are not distinguishable from each other.<sup>(421)</sup>

As was customary with him, Dirac first recast Schrödinger's theory in his own formalism. He noted the fact that, just as one might consider p and q as dynamical variables, one should also consider the negative energy -Eand the time t as variables corresponding to the differential relations

$$p_r = -i\frac{h}{2\pi}\frac{\partial}{\partial q_r}$$
 and  $-E = -i\frac{h}{2\pi}\frac{\partial}{\partial t}$  (188)

He had already introduced this step a few months earlier in a paper on

"Relativity Quantum Mechanics with an Application to Compton Scattering," where he talked about "quantum time" with a view to introducing relativity into quantum mechanics.<sup>(430)</sup> From Eq. (188) he drew two conclusions: first, that only rational integral functions of E and p have meaning; second, that one cannot multiply, in general, an equation containing the p's and E by a factor from the right-hand side. Dirac then rewrote the Schrödinger equation in the form

$$F(q_r, p_r, t, E) \psi = [H(q_r, p_r, t) - E] \psi = 0$$
(189)

remarking that Heisenberg's original quantum mechanics follows from a special choice of the eigenfunctions.

In Section 4 of the same paper,<sup>(428)</sup> dealing with the Schrödinger equation, Dirac proceeded to make another very important contribution by giving a general treatment of systems containing several identical particles. Dirac said that if there is a system with, say, two electrons, and one considers two states (mn) or, more accurately, (m(1), n(2)) and (m(2), n(1)), which are distinguished only by the fact that in the second state the two electrons have been interchanged, then according to his and Heisenberg's scheme, one has to count the two states as one.<sup>(431)</sup> With this counting procedure, however, one cannot easily describe functions which are antisymmetrical in the electron coordinates. The general expression for the two-particle eigenfunction is

$$\psi_{mn} = a_{mn}\psi_m(1)\psi_n(2) + b_{mn}\psi_m(2)\psi_n(1) \tag{190}$$

There exist, however, only two choices for the coefficients a and b. Either

$$a_{mn} = b_{mn}$$
 symmetrical case (Bose–Einstein statistics), (191)

or

 $a_{mn} = -b_{mn}$  antisymmetrical case (Fermi-Dirac statistics) (192)

The latter case follows from Pauli's exclusion principle which holds for electrons. He then went on to consider gases of free particles in a volume V, obeying either Bose-Einstein statistics or the statistics deduced from the exclusion principle. For a number  $N_s$  of particles in the sthe set (having the energy  $E_s$ ), he derived

$$N_s = \frac{A_s}{\exp\left(\frac{\alpha + E_s}{kT}\right) + 1}$$

where

$$A_s = 2\pi V (2m)^{3/2} E_s^{1/2} \frac{dE}{h^3}$$
(193)

and  $\alpha$  is related to the density.

Dirac's recognition of the new statistics was antedated by the work of Enrico Fermi, who had obtained the same result several months earlier.<sup>(432)</sup> As Dirac recalled: "I had read Fermi's paper about Fermi statistics and forgotten it completely. When I wrote up my work on the antisymmetric wave functions, I just did not refer to it at all. Then Fermi wrote and told me and I remembered that I had previously read about it.<sup>(433)</sup> At the time when Dirac read Fermi's paper, it did not strike him as being important and it completely slipped his mind. A few months later he rediscovered that result, and the new statistics has since then been called "Fermi-Dirac statistics." In his work, Dirac went beyond Fermi and linked the two statistics to the symmetry properties of the eigenfunctions. This was a most important point which had to do with a deeper discussion of the problem of identical particles. Dirac had not pondered about statistics until this problem became "pretty obvious" to him. When he saw the problem, however, he immediately found the solution. In all this, the Schrödinger function obviously helped him a lot and automatically led him to consider the symmetry properties of a function describing several identical particles. Another important factor in his new considerations, the exclusion principle, had also not concerned him before at all, but when he had to decide the question whether a wave function is symmetric or antisymmetric in the exchange of two-electron coordinates, he reminded himself of Pauli's rule.

# 17. TOWARDS AN UNDULATORY INTERPRETATION OF ATOMIC PHENOMENA; FURTHER APPLICATIONS OF WAVE MECHANICS

## 17.1. Early Expressions of Schrödinger's Undulatory View of Atomic Processes

The desire to develop an undulatory interpretation of atomic processes arose in Schrödinger as a result of his successful applications of Louis de Broglie's idea of matter waves: first to derive Einstein's theory of ideal gases and then to obtain a consistent description of the nonrelativistic hydrogen atom. Once the wave equation had been shown to yield the correct energy states of the hydrogen atom and, within this context, an

148

intuitive (*anschauliche*) explanation of the quantization condition—which Schrödinger thought to be an arbitrary and unnatural imposition on the dynamical equations of the electron—the question had to be asked as to what was really oscillating within the atoms. That is, historically, Schrödinger's wave equation did not grow out of his preconception of an undulatory description of atoms; rather, the evidently successful wave equation urgently demanded the development of such a description.

Schrödinger stated everything that he knew or considered on the subject of atomic eigenvibrations in his notebook on "Eigenwertproblem des Atoms. II," whether it led to a solution or not, and whether he used it or not in his later paper. The statements in the first communication of January 1926, such as, "It is, of course, strongly suggested that we should try to connect the function  $\psi$  with some vibration process in the atom, which would more nearly approach reality than the electronic orbits" and "I originally intended to found the new quantum conditions in this more intuitive manner," (434) should not be taken to indicate already the existence of such an "intuitive manner," but rather a future program which Schrödinger worked out piece by piece during the following several months, partly in connection with his attempt to provide a general foundation to wave mechanics, and partly in response to specific questions asked by his correspondents.

The "Hamiltonian analogy between mechanics and optics," which Schrödinger presented in Section 1 and applied to atomic theory in Section 2 of his second communication,<sup>(435)</sup> contains the earliest aspects of what he meant by this "intuitive" picture. Of course, we have to bear in mind that a formal or mathematical analogy between (classical or quantum-theoretical) atomic dynamics and the methods used to describe the behavior of optical systems is not the same as an undulatory interpretation of the former. The outlines of such an interpretation may be gathered from the following programmatic statements by Schrödinger:

The true mechanical process is realized or represented in a fitting way by the wave processes in [a non-Euclidean, many-dimensional] q-space.... A macroscopic mechanical process  $\cdots$  can approximately enough be regarded as confined to a point compared with the geometrical structure of the path.... This manner of treatment, however, loses all meaning where the structure of the path is no longer very large compared with the wavelength or indeed is comparable with it. Then we must treat the matter strictly on the wave theory, i.e., we must proceed from the wave equation and not from the fundamental equations of mechanics, in order to form a picture of the manifold of the possible processes.<sup>(436)</sup>

The crucial wavelength which limits the validity of the (classical) mechanical description had been provided by Louis de Broglie. Schrödinger remarked:

In *this* sense do I interpret the "phase waves" which, according to de Broglie, accompany the path of the electron; in the sense, therefore, that no special meaning is to be attached to the electronic path itself (at any rate, in the interior of the atom), and still less to the position of the electron on its path.<sup>(437)</sup>

Up to now Schrödinger's remarks concerning a wave interpretation associated with this wave equation formalism (and contained in the first two communications completed by the end of February 1926) did not proceed beyond the immediate visualization of the mathematical results. One thing appeared to be absolutely clear: "The  $\psi$ -vibrations are of course not electromagnetic vibrations in the old [classical] sense."<sup>(277)</sup> However, a relation had to exist between the matter vibrations and the Maxwell-Lorentz electromagnetic current, and Schrödinger suggested: "The  $\psi$ -vibrations must then corrrespond to the four-current, i.e., the [Maxwell-Lorentz] four-current must be replaced by something derived from the function  $\psi$ , say the four-dimensional gradient of  $\psi$ . But this is all pure fantasy; in reality, I have still not thought about it at all."<sup>(277)</sup>

On the other hand, Schrödinger had pondered on Sommerfeld's doubts concerning the physical reality of matter waves and arrived at the conclusion: "By the way, my general presentation [of wave mechanics in the second communication<sup>(256)</sup>] approaches your wishes on a second point, namely with respect to the physical reality of  $\psi$ -vibrations. Due to the fact that in general  $\psi$  depends on many more than three variables, the immediate interpretation [of the matter wave] in three-dimensional space is rendered difficult in any desirable manner."<sup>(277)</sup>

In a letter written to Erwin Schrödinger, the Munich experimentalist Wilhelm Wien praised the fact that the new theory had solved "the problem of atomic vibrations, and this fortunately in close connection with the classical theory."<sup>(438)</sup> He had evidently missed a close connection with the classical theory in the theoretical work on atomic physics of the past few years. In a footnote in his paper on the equivalence of his wave mechanics to the Göttingen quantum mechanics, Schrödinger supported Wien's point of view, when he emphasized: "I am not aware at all of any generic relation [of wave mechanics] with Heisenberg's [matrix mechanics]. I naturally knew about his theory, but I was discouraged (*abgeschreckt*), if not repelled (*abgestoßen*), by what appeared to me as very difficult methods of transcendental algebra, defying any visualization (*Anschaulichkeit*)."<sup>(439)</sup>

On March 19, 1926, after submitting the paper containing the formal equivalence between the wave and matrix mechanical methods,<sup>(439)</sup> Schrödinger reported to Wien happily that "the relationship with Heisenberg['s mechanics] is now completely clarified, namely in the sense that anybody who does not wish to calculate with matrices need not do so"; he

further emphasized: "As far as physics is concerned, my own theory definitely appears to me to be considerably more satisfactory and capable of extension, because one has visualizability (*Anschauung*) as a guide."<sup>(346)</sup>

These optimistic opinions notwithstanding, Schrödinger was only able to put forward some general points of view in favor of the "intuitiveness" of wave mechanics. These he summarized in Section 5 of the paper on equivalence under the title "Vergleich der beiden Theorien" ("Comparison of the Two Theories").<sup>(349)</sup> Schrödinger noted that matrix mechanics "does not tempt us, due to the complete absence of visualizability (Anschauung), to form space-time pictures of what happens in atoms; pictures, which must perhaps, remain uncontrollable in principle."<sup>(440)</sup> Still, the actual situation was not all that simple due to the formal equivalence between the corresponding mathematical expressions in the wave and matrix descriptions (which Schrödinger had himself shown). He explained: "The equivalence exists in reality, and it also exists in the reverse direction,<sup>(440)</sup> arguing that from the matrices one is able to construct eigenfunctions fully.<sup>(441)</sup> Hence it was possible, in principle, to derive from matrix mechanics the intuitive (anschauliche) pictures of wave mechanics by applying a clear mathematical procedure. In spite of this conclusion, Schrödinger added a warning, namely, "that the thesis that mathematical equivalence and physical equivalence are the same can, on the whole, be considered as having only restricted validity at all."<sup>(442)</sup> In particular, Schrödinger expected that wave mechanics alone was most likely capable of treating processes including the collision of atoms with electrons,  $\alpha$ -particles, or molecules. He claimed: "To approach [the theoretical description] of such problems, it is quite necessary to oversee clearly the transitions between the macroscopic, visualizable mechanics and the micromechanics of an atom.... To me it seems extraordinarily difficult to tackle problems of the kind mentioned above, as long, as we feel obliged on epistemological grounds to suppress intuition in atomic dynamics, and to operate only with such abstract concepts like transition probabilities, energy levels, etc."<sup>(443)</sup>

### 17.2. The "Real" Wave Equation and Time-Dependent Theory

On June 18, 1926, Erwin Schrödinger wrote to Wilhelm Wien: "I am just giving the final touches to the fourth communication, which I shall send off, if not tomorrow, then on Monday. With its completion several, quite heavy burdens are lifted from my heart: namely, first, the electrodynamical significance of  $\psi$  in the case of [systems of] more than three degrees of freedom; second, the definition of the concept of electric current density, which was indispensable in complementing the concept of charge density; and as a third point, last but not least, the coupling between the eigenvibrations and the electromagnetic field. That problem could be solved, for the moment at least, in the case of an *incident* [electromagnetic] wave, in a straightforward manner without involving any new assumptions. I hope that it will not be too difficult to generalize the treatment so as to take into account the back-coupling of the self-emitted wave [by the atomic system]—but I no longer wanted to keep back the results reached so far...."<sup>(444)</sup>

With these words of satisfaction Schrödinger informed Wien of the major progress he had achieved during the weeks since submitting his last, third communication on wave mechanics. This progress included new insights into several of the remaining problems of the undulatory description of atomic phenomena and, especially, an important generalization of the mathematical scheme of the theory. The heart of this scheme was a new wave equation, which has sometimes been called "Schrödinger's second equation." As Eugene Wigner recalled six decades after the appearance of this equation: "Schrödinger's 'second equation' was immensely important even though it was little emphasized by him or, actually, by anybody else at the time it appeared. But it was soon very generally recognized—it gave quantum mechanics a much more general, and *much* more traditional, basis than the original, given by Heisenberg [: quantum mechanics gave the energy levels and transition probabilities]. I recall how much I was delighted when reading and understanding it."<sup>(445)</sup>

Wigner recognized—in the fourth communication (Part IV) of Schrödinger's series on wave mechanics—nothing other than a *second*, *fundamental* wave equation; and he claimed that it was actually this equation which eventually deepened and generalized the basis of the new atomic theory beyond that which Heisenberg and his collaborators had already obtained and Schrödinger, with his "first" wave equation, had only confirmed. How did Schrödinger, the creator of the second wave equation, judge the situation in June 1926?

Schrödinger explained the necessity of generalizing the previous theory, right at the beginning of the fourth communication in quite some detail. The old wave equation (of Parts I and II), notably

$$\Delta \psi - \frac{2(E-V)}{E^2} \frac{\partial^2 \psi}{\partial t^2} = 0$$
(194)

or

$$\Delta \psi + \frac{8\pi^2}{h^2} (E - V) \psi = 0$$
 (195)

(where E is the total energy, V is the potential energy of the system under consideration, and h is Planck's constant), he argued, "suffers from the dis-

advantage that it expresses the law of variation of the 'mechanical field scalar'  $\psi$ , neither *uniformly* nor *generally*."<sup>(446)</sup> These equations hold, in particular, only for a given energy of the system under investigation; hence the time-dependence of  $\psi$  described by the undulatory theory developed so far is restricted to a periodic factor

$$\psi = \psi_0(x) \exp\left(\pm \frac{2\pi i}{h} Et\right)$$
(196)

and consequently the wave equation reduces to an equation for the *amplitude*  $\psi(x)$ , with x denoting the space variables. This fact restricts the applicability of the theory to those atomic systems whose potential energy does not depend explicitly on time, i.e., to conservative systems. Schrödinger then wrote: "There arises, however, an urgent need for the extension of the theory to nonconservative systems, because it is only in that way that we can study the behavior of a system under the influence of prescribed external forces, e.g., a light wave, or a strange atom flying past."<sup>(447)</sup> For that purpose, he argued, one must abandon the amplitude equation and "search for the real wave equation."<sup>(447)</sup>

In order to obtain the "real" equation, one may depart from the identity

$$\frac{\partial^2 \psi}{\partial t^2} = -\frac{4\pi^2 E^2}{h^2} \psi \tag{197}$$

which is valid for conservative systems, and insert it into Eq. (195). Thus one arrives at the higher-order wave equation

$$\left(\Delta - \frac{8\pi^2}{h^2}V\right)^2\psi + \frac{16\pi^2}{h^2}\frac{\partial^2\psi}{\partial t^2} = 0$$
(198)

which should be valid for "every  $\psi$  which depends on time as in [Eq. (196)], though with E arbitrary, and consequently also for every  $\psi$  which can be expanded in a Fourier series with respect to the time."<sup>(447)</sup> Now Schrödinger claimed: Eq. [(196)] is thus evidently the uniform and general wave equation for the field scalar  $\psi$ ."<sup>(448)</sup>

Schrödinger was not afraid of the mathematical complications of higher-order equations; the methods of their solution were well known in principle and treated, for example, in the book by Courant and Hilbert.<sup>(449)</sup> Moreover, he saw immediately that Eq. (198), in the case of time-independent potentials V, could be written simply as

$$\left(\Delta - \frac{8\pi^2}{h^2}V + \frac{8\pi^2}{h^2}E\right)\left(\Delta - \frac{8\pi^2}{h^2}V - \frac{8\pi^2}{h^2}E\right)\psi = 0$$
(199)

that is, a decomposition into the original, second-order equation (195) was possible.  $^{(450)}$ 

In the case of the time-dependent cases, it was possible to write a second-order differential equation by considering the fact that the time dependence of the wave equation might be expressed not by the second-order differential equation (197) but rather by the linear relation

$$\frac{\partial \psi}{\partial t} = \pm \frac{2\pi i}{h} E \psi \tag{200}$$

When one used this relation in conjunction with Eq. (195), the secondorder wave equation

$$\Delta \psi - \frac{8\pi^2}{h} V \mp \frac{4\pi i}{h} \frac{\partial \psi}{\partial t} = 0$$
(201)

resulted. The price one had to pay was that the wave function  $\psi$  satisfying Eq. (201) definitely became a *complex* object. Schrödinger now declared that Eq. (201) constituted the "real wave equation" and took it as the basis of his further considerations of atomic systems.

The applications of the new, "second equation" covered Sections 2-5 of Schrödinger's fourth communication.<sup>(446)</sup> However, instead of developing the most general time-dependent scheme, Schrödinger restricted himself essentially to treating dispersion phenomena, i.e., the interaction of external radiation with atoms. Of course, the dispersion phenomena represented important physical examples and had played a crucial role in recent quantum-theoretical investigations; in Schrödinger's opinion, they were also supposed to throw light on the "coupling between the eigenvibrations [of the atom] and the atom and the electromagnetic field," the crucial question emphasized repeatedly in his letters to Wilhelm Wien. The preference for first applying the time-dependent theory to dispersion phenomena was not a unilateral decision by Erwin Schrödinger, but would soon be shared by Paul Dirac. In Section 5 of his paper "On the Theory of Quantum Mechanics"-which was submitted before Schrödinger's fourth communication appeared in print-Paul Dirac sketched independently a timedependent perturbation theory of wave mechanics.<sup>(428)</sup> He immediately used this formalism to calculate the equilibrium of radiation and atoms,<sup>(451)</sup> but in later papers he turned to dealing with more genuine dispersion phenomena.<sup>(452)</sup>

In his letter to Erwin Schrödinger, dated June 23, 1926, Wilhelm Wien reassured his colleague that he considered wave mechanics an important step toward a final solution of the quantum problem. He wrote: "It is remarkable what you have achieved in a short time."<sup>(453)</sup> Wien had heard

from Sommerfeld—who had just returned from a visit to Zurich<sup>(444)</sup>—that Schrödinger was seriously contemplating passing through Munich in early July; thus he added in his letter: "All the physicists in Munich would really be delighted, since we then hope to have your theory presented to us by you, instead of by [Constantin] Carathéodory and [Gregor] Wentzel—for only those who have already studied your papers can understand their presentation."<sup>(453)</sup>

From the spring of 1926, Max Planck in Berlin and Wilhelm Wien and Arnold Sommerfeld in Munich had repeatedly invited Erwin Schrödinger to come to Berlin and Munich, respectively, and speak on his new atomic theory. Schrödinger, who was extremely happy about the appraisal and approval that his work had received in both places, actually fulfilled these pressing and welcome invitations as soon as he could free himself from the obligations of the summer semester in Zurich. He first travelled to Berlin and spoke before the Physical Society on July 16 on the "Grundlagen einer auf Wellenlehre Begründeten Atomphysik" ("Foundations of an Atomic Physics Based on Wave Theory").<sup>(454)</sup> He stayed on in Berlin for a few days, as a personal guest of Max Planck, and then he returned to Zurich via Munch. In Munich he delivered a similar lecture, entitled "Grundlagen einer auf Wellenlehre begründeten Atomphysik" ("Basic ideas of an Atomic Physics Founded on Wave Theory") to the Bavarian Section (Gauverein) of the German Physical Society on July 23, 1926.<sup>(455)</sup>

The time was indeed ripe for a first review of wave mechanics by its creator. Schrödinger had especially available the results of his fourth communication, in which the theory had received an important generalization and—as it seemed to Schrödinger—a reasonably *anschauliche* interpretation also. Since no manuscript or publication exists of the Berlin and Munich lectures, we do not know in detail the topics he discussed there. However, about a month later (on September 3, 1926) Schrödinger signed a paper in English, entitled "An Undulatory Theory of the Mechanics of Atoms and Molecules" and submitted it to the *Physical Review*, where it appeared in the December issue.<sup>(456)</sup> It can safely be assumed that this review (for the American public) essentially contained the material of the Berlin and Munich talks. Hence we shall reproduce here the titles of the sections as given in the paper's extract:

- 1. The Hamiltonian analogy between mechanics and optics.
- 2. The analogy is to be extended to include real "physical" or "undulatory" mechanics instead of mere geometrical mechanics.
- 3. The significance of wavelength; macromechanical and micromechanical problems.
- 4. The wave equation and its application to the hydrogen atom.

- 5. The intrinsic reason for the appearance of discrete characteristic frequencies.
- 6. Other problems; intensity of emitted light.
- 7. The wave equation derived from a Hamiltonian variation principle; generalization to an arbitrary conservative system.
- 8. The wave function physically means and determines a continuous distribution of electricity in space, the fluctuations of which determine the radiation by the laws of ordinary electrodynamics.
- 9. Nonconservative systems. Theory of dispersion and scattering and of the "transitions" between the "stationary states."
- 10. The question of relativity and the action of a magnetic field. Incompleteness of that part of the theory.<sup>(457)</sup>

From these contents it becomes evident that Schrödinger covered in his review all the results he had hitherto obtained in his main communications.<sup>(244,256,379,446)</sup> Interestingly enough, he left out a closer discussion of the formal equivalence of the undulatory and matrix mechanics.<sup>(349)</sup> But, psychologically, in a review advocating "the extreme conception"<sup>(457)</sup> of wave mechanics, such an omission of matrix mechanics may have been well motivated. In any case, Schrödinger advocated the new theory by pointing out the following "chief advantages":

- (a) The laws of motion and the quantum conditions are deduced simultaneously from one simple Hamiltonian principle.
- (b) The discrepancy hitherto existing in quantum theory between the frequency of motion and the frequency of emission disappears insofar as the latter frequencies coincide with the differences of the former. A definite localization of the electric charge in space and time can be associated with the wave system and this with the aid of ordinary electrodynamics accounts for the frequencies, intensities, and polarizations of the emitted light and makes super-fluous all sorts of correspondence and selection principles.
- (c) It seems possible by the new theory to pursue in all detail the so-called "transitions," which up to now have been wholly mysterious.
- (d) There are several instances of disagreement between the new theory and the older one as to the particular values of energy or frequency levels. In these cases it is the new theory that is better supported by experiment.<sup>(458)</sup>

What were the difficulties of his theory that Schrödinger had pointed out? In his account for the *Physical Review*, he mentioned the incompleteness of the relativistic and magnetic part of wave mechanics, in particular, the fact that the well-known fine-structure formula for hydrogen did not come out. "The deficiency must be intimately connected with Uhlenbeck-Goudsmit's theory of the spinning electron," he suggested finally, and added: "But in what way the electron spin has to be taken into account in the present theory is yet unknown."<sup>(459)</sup> Another difficulty, mainly of conceptual understanding, can be seen by looking at the end of the fourth communication. There, Schrödinger had stated: "Meantime, there is no doubt a certain crudeness in the use of a *complex* wave function. If it were unavoidable in principle, and not merely a facilitation of the calculation, this would mean that there are in principle two wave functions, which must be used together in order to obtain information on the state of the system."<sup>(460)</sup> However, he hoped that the complexity of the wave function existed in a formal way only and might be replaced perhaps by a real wave function and its time derivative, a possibility which he considered to be "the very much more congenial (sympathischere) interpretation."<sup>(460)</sup> At that moment this question could not be decided, because Schrödinger had not yet succeeded in replacing Eq. (201)-which introduced the complexity of the wave function-with a suitable real fourth-order equation for nonconservative or time-dependent systems.

How did Schrödinger's audience react to his presentation of the theory? In general, the physicists in Berlin, especially Max Planck and Albert Einstein, were very impressed. Einstein, for example, wrote to Arnold Sommerfeld: "Of the new attempts to obtain a deeper formulation of the quantum laws, I like that of Schrödinger most. If only the undulatory fields introduced by it could be transplanted from the *n*-dimensional coordinate space into the three- or four-dimensional one, respectively!"<sup>(461)</sup>

As far as the Munich lecture is concerned, we have the report of Werner Heisenberg, the originator of the competing atomic theory. Many decades later, Heisenberg vividly recalled Schrödinger's colloquium and the discussion afterwards. Thus, for instance, he related in 1968:

In July 1926 Schrödinger was invited to Munich by Wilhelm Wien to report on his theory. The experimental physicists in Munich, headed by Wien, were enthusiastic about the possibility that now perhaps this whole "quantum mystery of atomic physics" might be dealt with, and one would be able to return to the classical concept of honest fields, such as one had learned from Maxwell's [electromagnetic] theory. I listened to this lecture by Schrödinger, as I was then staying with my parents in Munich for the vacation; and I was then really quite horrified by his interpretation, because I simply could not believe it. I objected in the discussion that with such an interpretation one would not even be able to explain Planck's heat radiation law. But general opinion at that time was extremely hostile toward my objection. Wien answered me very harshly in that he could understand that now I felt sad about the fact that the whole quantum jumping, the matrices and all that had become superfluous; but it would be better, anyway, for me to leave the field to Schrödinger, who would certainly solve all the difficulties in the [near] future. This was not very encouraging; I did not have the slightest chance to get across my point of view in the discussion.<sup>(462)</sup>

One of the reasons for the unpleasant encounter between Heisenberg and Wien (after Schrödinger's lecture at Munich) must be sought in the earlier history of the Heisenberg-Wien relations. Back in July 1923, Heisenberg had practically failed in the experimental part of the examination for his doctorate with Wien. At that time, Wilhelm Wien had formed the opinion that the young candidate had not learned "decent physics" seriously enough. Moreover, the later development of atomic theory, in which Heisenberg played an increasingly important role, did not impress Wien favorably. He certainly had people like Heisenberg in mind when he wrote to Schrödinger, before the latter's visit to Munich, that he had not only disliked the erstwhile status of atomic theory and had stopped following it, but also: "Not least was I worried that the young physicists no longer realize what one is really looking for from a physical theory."<sup>(453)</sup> Wien had declared that the "quagmire of integral and half-integral quanta, of discontinuities and of arbitrary use of the classical theory," in short, all that had been dear to Heisenberg from the beginning of his studies in atomic theory, was not decent physical theory, and he urgently desired that the young quantum physicists "soon become used to rigorous physical thinking again."<sup>(453)</sup>

No, Heisenberg defintely had no chance of making any point during that discussion in July 1926. On the other hand, as he recalled later, he was not alone and isolated in Munich. At least Sommerfeld shared his main conclusions, as he wrote in a letter to Wolfgang Pauli shortly after the event: "We have had Schrödinger here, together with Heisenberg. My general impression is this, although "wave mechanics" is an admirable micromechanics, the fundamental quantum riddles, however, are not solved by it in the least. For the time being I don't believe Schrödinger anymore, from the instant where he starts to calculate with the  $c_k$  (the amplitudes of the different simultaneous eigenvibrations)."<sup>(463)</sup> It seems that either Sommerfeld did not elaborate on this point in the discussion of Schrödinger's talk in Munich, or Heisenberg did not remember; however, he did recall that he wrote a sad ("*traurigen*") letter to Niels Bohr, upon which "Bohr invited Schrödinger to Copenhagen for discussions in September of the same year."<sup>(462)</sup>

### 17.4. The Relativistic and Magnetic Field Equation

When Erwin Schrödinger embarked upon the undulatory treatment of the hydrogen atom in November 1925, he aimed at a complete relativistic theory. Indeed, the first wave equation that he wrote (in the three-page manuscript on "*H-Atom. Eigenschwingungen*") was a relativistic wave equation, namely,

$$\Delta \psi = -\frac{4\pi^2 v^2}{u^2} \psi = \frac{4\pi^2}{h^2} m^2 c^4 \left[ \left( \frac{hv}{mc^2} + \frac{e^2}{mc^2 r} \right)^2 - 1 \right] \psi$$
(202)

It was not only disagreement between the energy states calculated from this equation and the experimentally obtained hydrogen terms that forced Schrödinger to restrict his initial publications to the nonrelativistic approximation. Nevertheless, the unpublished manuscripts, as well as occasional hints in published papers, amply demonstrate how incessantly Schrödinger thought about the relativistic extension of the atomic wave equation in the following months.

Schrödinger ultimately presented the relativistic wave equation by translating directly the classical Hamilton-Jacobi partial differential equation for an electron (charge e and mass m), namely,

$$\left(\frac{1}{c}\frac{\partial W}{\partial t} + \frac{e}{V}\right)^2 - \left(\frac{\partial W}{\partial x} - \frac{e}{c}A_x\right)^2 - \left(\frac{\partial W}{\partial y} - \frac{e}{c}A_y\right)^2 - \left(\frac{\partial W}{\partial z} - \frac{e}{c}A_z\right)^2 - m^2c^2 = 0$$
(203)

according to the rules of time-dependent theory. In Eq. (203), V and  $A_x, A_y, A_z$  denote the electromagnetic potentials at the position of the electron and W the (characteristic) action function. Upon squaring the expressions on the left-hand side and making the replacements

$$\frac{\partial W}{\partial t} \rightarrow \pm \frac{h}{2\pi i} \frac{\partial}{\partial t}, \qquad \frac{\partial W}{\partial x} \rightarrow \pm \frac{h}{2\pi i} \frac{\partial}{\partial x}$$

$$\frac{\partial W}{\partial y} \rightarrow \pm \frac{h}{2\pi i} \frac{\partial}{\partial y}, \qquad \frac{\partial W}{\partial z} \rightarrow \pm \frac{h}{2\pi i} \frac{\partial}{\partial z}$$
(204)

one obtains the wave equations  $(A = (A_x, A_y, A_z))$ 

$$\begin{aligned} & \Delta \psi - \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} \mp \frac{4\pi i e}{h c} \left( \frac{V}{c} \frac{\partial \psi}{\partial t} + A \operatorname{grad} \psi \right) \\ & + \frac{4\pi^2 c^2}{h^2 c^2} \left( V^2 - A_x^2 - A_y^2 - A_z^2 - \frac{m^2 c^4}{c^2} \right) \psi = 0 \end{aligned} \tag{205}$$

Schrödinger concluded: "The pair of equations [(205)] would be the possible relativistic-magnetic generalization [of the time-dependent non-relativistic equations] for the single electron, and should be likewise understood to mean that the complex wave function has to satisfy either the one or the other equation."<sup>(464)</sup> The introduction of the complex wave function enabled one to write, as in the nonrelativistic case, a second-order wave equation. Evidently, the purely relativistic fine structure should result by putting the electromagnetic potentials in Eq. (205) equal to zero.

The wave equation thus essentially completed, at least for the oneelectron problem, Schrödinger's program of an undulatory description of the atoms. By the time it appeared in print (in a September issue of the *Annalen der Physik*), however, several other authors had independently arrived at the same generalization of the wave equation. Thus the relativistic equation (205)—or its special case with zero potentials—would later be associated with different names, notably those of Oskar Klein and Walter Gordon, but occasionally also with others. In order to understand the reason for this custom, we shall give here a condensed review of how the various physicists proceeded and what explicit results they found. It must be emphasized strongly, however, that all of them were motivated by Schrödinger's first publications on wave mechanics.

The purest form of the Klein-Gordon equation occurred first perhaps in a letter by Wolfgang Pauli, the same one which he had written to Pascual Jordan on the equivalence of Schrödinger's undulatory methods with those of matrix mechanics. Thus he introduced the expressions for the momentum p and the energy E of a relativistic particle of mass m into what he called the "wave equation of de Broglie's radiation field," i.e., the timedependent wave equation, where u = E/p. Thus there followed immediately the wave equation

$$\Delta \psi - \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} + \frac{m^2 c^2}{E^2} \frac{\partial^2 \psi}{\partial t^2} = 0$$
(206)

Pauli also wrote in his letter the equation of a particle in a potential, that is, essentially Schrödinger's later Eq. (205).<sup>(465)</sup>

As far as the date of publication is concerned, Oskar Klein was the first to concern himself with the relativistic wave equation. Since the early 1920s Klein had been a member of the inner circle around Bohr and had already contributed several important results to atomic theory. In his paper on "Quantum Theory and Five-Dimensional Relativity Theory," which Klein submitted in late April 1926 to *Zeitschrift für Physik*,<sup>(466)</sup> he claimed to have found "a simple relationship between the theory proposed by [Theodor] Kaluza<sup>(467)</sup> for the connection between electromagnetism and

gravitation, on the one hand, and the method given by [Louis] de Broglie<sup>(218)</sup> and [Erwin] Schrödinger<sup>(244,256)</sup> for treating quantum problems, on the other hand."<sup>(468)</sup> Klein considered the following differential equation in five-dimensional space,

$$\sum_{i,k} a^{ik} \left( \frac{\partial^2 U}{\partial x^i \partial x^k} - \sum_r \begin{bmatrix} ik \\ r \end{bmatrix} \frac{\partial U}{\partial x^r} \right) = 0$$
(207)

involving the (five-dimensional) three-index symbols—a generalization of the symbols in general relativity theory, with the metric tensor  $\gamma_{ik}$  replacing  $g_{ik}$ —and a symmetric tensor  $a^{ik}$  whose components depended on the coordinates. Further, he considered this equation as a wave equation in the sense of de Broglie and Schrödinger. From the fundamental equation (207), Klein derived—in the special case of retaining only the electrostatic field (i.e.,  $\Phi_1 = \Phi_2 = \Phi_3 = 0$ , where  $\Phi_1 = A_x$ ,  $\Phi_2 = A_y$ ,  $\Phi_3 = A_z$ ,  $-(\frac{1}{c}) \Phi_4 = V$  are the components of the electric four-vector)—the second-order wave equation

$$\Delta U - \frac{1}{c^2} \frac{\partial^2 U}{\partial t^2} - \frac{2eV}{c^2} \frac{\partial^2 U}{\partial t \, \partial x^0} + \left(m^2 c^2 - \frac{e^2 V^2}{c^2}\right) \frac{\partial^2 U}{\partial x^{0^2}} = 0$$
(208)

Since, for an electron, U may be written as

$$U = \exp\left[-2\pi i \left(\frac{x^0}{h} - vt\right)\right] \psi(x, y, z)$$
(209)

Eq. (208) reduces to the original Schrödinger equation<sup>(469)</sup>

$$\Delta \psi + \frac{4\pi^2}{c^2 h^2} \left[ (hv - eV)^2 - m^2 c^4 \right] \psi = 0$$
(210)

The next publication on the relativistic generalization of the Schrödinger equation came from Leningrad. Vladimir Fock had read Schrödinger's first two communications in *Annalen der Physik*, and noticed his difficulties in obtaining the correct relativistic extension; he therefore tried "to remove some of these difficulties and to derive the wave equation in question for the general case of a Lagrange function [describing atomic systems] having linear terms."<sup>(470)</sup> Departing from the time-dependent Hamilton–Jacobi equation describing a relativistic system having f degrees of freedom,

$$H\left(q_{i},\frac{\partial W}{\partial p_{i}}\right) + \frac{\partial W}{\partial t} = 0$$
(211)

Fock obtained—in the case of the Zeeman effect, where a magnetic field H acts along the z-direction—the wave equation

Fock solved Eq. (212) with the help of spherical coordinates for the space dependence of the wave function  $(\psi = \psi_1(x, y, z) \exp[(2\pi i/h) Et]$  and obtained the normal Zeeman effect. [In Eq. (212), E is the energy parameter, m and e denote the mass and absolute charge of the electron, and c is the velocity of light *in vacuo*.]

Several weeks later, in late July 1926, Fock submitted another paper on the subject, entitled "On the Invariant Form of the Wave Equation and the Equations of Motion of a Charged Mass Point," to the *Zeitschrift für Physik*.<sup>(471)</sup> In this paper, Fock presented, first, the explicit form of the relativistic equation for a charged particle, his result agreeing with Schrödinger's result in Eq. (205); second, he developed a five-dimensional generalization of that wave equation, which had a structure similar to Klein's Eq. (207).

While Fock first searched directly for an extension of Schrödinger's wave equation in special relativity, Théophile De Donder, with Frans Henri van den Dungen, in Brussels, proposed a further approach within the scheme of general relativity.<sup>(472)</sup> In particular, they found that the gravitational interaction in general relativity might be described by an integral equation of the Fredholm type (in a generalized space due to the number of degrees of freedom of the system of particles considered), whose solution seemed to imply a periodic phenomenon that exhibited similarity to the undulatory behavior of microscopic particles in Schrödinger's wave mechanics. Later, De Donder carried this idea further in order to derive the quantum-theoretical behavior of an electron moving simultaneously in gravitational and electromagnetic fields.<sup>(473)</sup> He obtained a complicated wave equation whose nongravitational part coincided perfectly with Schrödinger's Eq. (205).

Equation (205) had, however, already appeared in an earlier issue of the *Comptes Rendus* of the Paris Academy of Sciences. It did so in a note entitled "Remarks on the New Undulatory Mechanics," which was presented at the meeting of the Academy on July 26, 1926; its author was Louis de Broglie, who considered the nonrelativistic wave equations of Schrödinger's previous communications—the fourth communication was not yet available in print—to be unsatisfactory.<sup>(474)</sup>

The Hungarian Janos Kudar from the University of Szeged also derived Eq. (205).<sup>(475)</sup> Walter Gordon in Berlin, in his paper on "The Compton Effect According to Schrödinger's Theory,"<sup>(476)</sup> which was received by Zeitschrift für Physik on September 29, 1926, presented a straightforward procedure for obtaining the relativistic wave equation for a massive, charged, microscopic particle moving in external electric and magnetic fields. Gordon did not refer to Schrödinger's fourth communication, which came out in print at just about the time when he finished his work and which contained parts of his results. Gordon departed from the classical equation for a relativistic charged particle (electron) with fourmomentum  $p_{\alpha}$  ( $\alpha = 1, 2, 3, 4$ ) in an electromagnetic field describe by the four-potential  $\Phi_{\alpha}$  ( $\alpha = 1, 2, 3, 4$ ), i.e.,

$$\sum_{\alpha} \left( p_{\alpha} - \frac{e}{c} \Phi_{\alpha} \right)^2 + m^2 c^2 = 0$$
(213)

By replacing energy and momentum variables by operators according to Schrödinger's rules  $(p_k \rightarrow (h/2\pi i)(\partial/\partial x_k)$  and  $E \rightarrow -(h/2\pi i)(\partial/\partial t))$ , Gordon obtained the wave equation

$$\left[\sum_{\alpha} \left(\frac{h}{2\pi i} \frac{\partial}{\partial x_{\alpha}} - \frac{e}{c} \Phi_{\alpha}\right)^{2} + m^{2}c^{2}\right] \psi = 0$$
(214)

After the procedure of squaring is carried out, the equation becomes

$$\sum_{\alpha} \frac{\partial^2 \psi}{\partial x_{\alpha}^2} - \frac{4\pi i e}{h c} \sum_{\alpha} \Phi_{\alpha} \frac{\partial \psi}{\partial x_{\alpha}} - \frac{4\pi^2}{h^2} \left( \frac{e^2}{c^2} \sum_{\alpha} \Phi_{\alpha}^2 + m^2 c^2 \right) \psi = 0$$
(215)

which coincides completely with Eq. (205)—with the upper sign—if one takes into account the strictly relativistic notation in Eq. (215); in particular, we have  $\Phi_1 = A_x$ ,  $\Phi_2 = A_y$ ,  $\Phi_3 = A_z$ , and  $\Phi_4 = iV$ . The work of Walter Gordon thus provided the most condensed mathematical presentation of the various versions of Schrödinger's equation, especially of the fully relativistic form; even though he was nearly the last to publish the results, this fact justifies the association of his name with Eq. (215) or its special case in the absence of electromagnetic potentials. Finally, Gordon did not stop at the relativistic wave equation, but went on to use it in a crucial problem: to calculate the Compton effect in wave mechanics. Oskar Klein—who, besides Schrödinger, first worked on the relativistic wave equation—and Walter Gordon are indeed the appropriate patrons of the equation that bears their names; this does not in any way minimize the fine contributions of Pauli, de Broglie, Fock, De Donder, and Kudar.<sup>(477)</sup>

### 17.5. Schrödinger's Visit to Copenhagen

From the very beginning. Heisenberg had been seriously opposed to Schrödinger's "anschauliche" interpretation of wave mechanics. Thus, for instance, he had written to Wolfgang Pauli in June: "The more I ponder on the physical part of Schrödinger's theory, the more detestable I find it. One should imagine the rotating electron, whose charge is distributed over the entire space and which has an axis in a fourth and fifth dimension. What Schrödinger writes on the visualizability of his theory ... I find rubbish. The great achievement of Schrödinger's theory is the calculation of matrix elements."<sup>(478)</sup> Schrödinger's colloquium in Munich had merely confirmed Heisenberg's negative opinion. A few days after the colloquium, he wrote to Pauli: "As nice as Schrödinger is personally, I find his physics so strange: one feels 26 years younger when listening to it. Indeed, Schrödinger throws overboard everything which is 'quantum-theoretical': namely. the photoelectric effect, the Franck[-Hertz] collisions, the Stern-Gerlach effect, etc. It is not then difficult to establish a theory [of the kind Schrödinger has in mind]. However, it does not agree with experience."<sup>(479)</sup> But the unfortunate discussion following Schrödinger's Munich lecture persuaded Heisenberg of the necessity of having a really detailed and penetrating discussion with Erwin Schrödinger elsewhere, most profitably in Copenhagen where Niels Bohr especially could participate.

In a letter dated September 11, 1926, Bohr actually invited Schrödinger to come to Copenhagen and deliver a lecture to the Danish Physical Society (Fysisk Forening) on wave mechanics. At the same time Bohr expressed the hope "that you will introduce some discussions for the narrower circle of those who work here at the Institute, and in which we can deal more deeply with the open questions of atomic theory."(480,481) Among this narrower circle belonged, in particular, Werner Heisenberg-from May, 1926 the main "Assistent" and "Lektor" at the Copenhagen Institute for Theoretical Physics-and Oskar Klein; Paul Dirac was also present at Bohr's Institute at that time. Schrödinger accepted Bohr's invitation quite readily, (482) and announced his arrival in Copenhagen on October 1.<sup>(483)</sup> There he was received with great eagerness: thus Heisenberg recalled: "Bohr's discussions with Schrödinger began at the railway station and were continued daily from early morning until late at night. Schrödinger stayed at Bohr's house so that nothing would interrupt the conversations."<sup>(484)</sup>

No contemporary notes about the content of the Copenhagen discussions exist; it does not seem to have occurred to anyone-neither Bohr. nor Schrödinger, nor any of the other participants-to keep such notes. Heisenberg later gave many lively accounts of the However. discussions.<sup>(485)</sup> As Heisenberg recalled, in Copenhagen Schrödinger especially attacked the idea of sudden quantum jumps. Schrödinger believed that the idea of quantum jumps was bound to end in nonsense. He reminded Bohr that "according to his (Bohr's) theory, if an atom is in a stationary state, the atom revolves periodically but does not emit light, when, according to Maxwell's theory, it must. Next the electron is said to jump from one orbit to the next and to emit radiation. Is this jump supposed to be gradual or sudden? If it is gradual, the orbital frequency and energy of the electron must change gradually as well. But in that case, how do you explain the persistence of fine spectral lines? On the other hand, if the jump is sudden. Einstein's idea of light quanta will admittedly lead us to the right wave number, but then we must ask ourselves how precisely the electron behaves during the jump. Why does it not emit a continuous spectrum, as electromagnetic theory demands? And what laws govern its motion during the jump? In other words, the whole idea of quantum jumps is sheer fantasy."<sup>(484)</sup>

Bohr agreed with Schrödinger's objections, but pointed out that they did not prove that there are no quantum jumps; only we cannot imagine them and the concepts with which we describe events in daily life and experiments in classical physics are inadequate when it comes to describing quantum jumps. "Nor should we be surprised to find it so," Bohr said, "seeing that the processes involved are not the objects of direct experience." (484) Schrödinger countered by saying that "if there are electrons in the atom, and if these are particles-as all of us believe-then they must surely move in some way. Right now I am not concerned with a precise description of this motion, but it ought to be possible to determine the principle of how they behave in the stationary state or during the transition from one state to the next. But from the mathematical form of wave or quantum mechanics alone, it is clear that we cannot expect reasonable answers to these questions. The moment, however, that we change the picture and say that there are no discrete electrons, only electron waves or waves of matter, then everything looks quite different. We no longer wonder about the fine lines. The emission of light is as easily explained as the transmission of radio waves through the aerial of the transmitter, and what seemed to be insoluble contradictions have suddenly disappeared."<sup>(484)</sup> Bohr disagreed with this and pointed out that the contradictions did not disappear: "You speak of the emission of light by the atom or more generally of the interaction between the atom and the surrounding radiation field, and you think that all the problems are solved once we assume that there are material waves but no quantum jumps. But just take the case of thermodynamic equilibrium between the atom and the radiation field—remember, for instance, the Einsteinian derivation of Planck's radiation law. The derivation demands that the energy of the atom should assume discrete values and change discontinuously from time to time; discrete values for the frequencies cannot help us here. You can't seriously be trying to cast doubt on the whole basis of quantum theory."<sup>(484)</sup>

Schrödinger conceded that all these relationships had not yet been fully explained, but pointed out that Bohr and his associates had also so far failed to discover a satisfactory physical interpretation of quantum mechanics. Bohr agreed that there were inconsistencies, as for example when one watched sudden flashes of light on a scintillation screen or the sudden rush of an electron through a cloud chamber; one could not just ignore these observations as if they did not exist at all.

On Bohr's defense of the concept of quantum jumps as being essential in describing the behavior of atoms and radiation, Schrödinger became quite despondent, and finally exclaimed: "If all this quantum jumping were here to stay, I should be sorry I ever got involved with quantum theory." To which Bohr replied: "But the rest of us are extremely grateful that you did; your wave mechanics has contributed so much to the mathematical clarity and simplicity that it represents a gigantic advance over all previous mechanics."<sup>(484)</sup>

Heisenberg also recalled that the continuous, strenuous discussions and conversations with Bohr exhausted Schrödinger. "After a few days Schrödinger fell ill, perhaps as a result of his enormous effort; in any case, he was forced to keep to his bed with a feverish cold. While Mrs. Bohr nursed him and brought in tea and cake, Niels Bohr sitting on the edge of the bed talking to Schrödinger: 'But you must surely admit that....'"(484) In other words Bohr-whom Heisenberg described as having been "an almost remorseless fanatic"<sup>(484)</sup> in the debate with Schrödinger-still had to convince his miserable guest to accept the Copenhagen position. However, "no real understanding could be expected since, at that time, neither side was able to offer a complete and coherent interpretation of quantum mechanics. For all that, we in Copenhagen felt convinced toward he end of Schrödinger's visit that we were on the right track, though we fully realized how difficult it would be to convince even leading physicists that they must abandon all attempts to construct perceptual models of atomic processes."<sup>(484)</sup>

Schrödinger, who delivered his lecture entitled "Grundlagen der undulatorischen Mechanik" ("Foundations of an Undulatory Mechanics") before the Danish Physical Society on October 4, 1926, stayed in Copenhagen only a few days. A couple of weeks later he reported to Wilhelm Wien: "...it was very nice that I was able to become thoroughly acquainted with Bohr-whom I had never known before-in his own surroundings, and to talk with him for hours about these matters which are so very dear to all of us."<sup>(486)</sup> In his letter to Wien, Schrödinger briefly sketched the contents of discussions in Copenhagen, especially the points of disagreement. He wrote: "Quite certainly, the point of view of [using] visualizable pictures, which de Broglie and I assume, has not been carried through nearly far enough in order to render an account of the most important facts [of atomic theory]. It is of course probable that here and there a wrong path was taken that must now be abandoned. But that, even if one is Niels Bohr, one could possibly say at this point: the visualizable wave pictures work as little as the visualizable point [-particle] models, there being something in the results of observation which cannot be grasped by our erstwhile way of thinking; this I do not believe. I believe it even less since for me the comprehensibility of the external processes in nature is an axiom, say, in the sense: to grasp experience means nothing more than establishing the best possible organization among the different facts of experience."<sup>(486)</sup> In Schrödinger's opinion, the facts of experience could not contradict each other, as Bohr-for many years-had tended to assume in atomic physics; only the "theoretical connections" ("gedankliche Verbindungsglieder") or the physical interpretations could do so. In particular, it seemed "premature" ("voreilig") to give the "completely general conceptions of space and time and the connection of the interaction of neighboring space-time points," concepts that had been preserved even in general relativity theory.<sup>(486)</sup>

Schrödinger further remarked to Wien: "I can only say that I don't care at all for this whole play of waves, if it should turn out to be nothing more than a comfortable computational device to evaluate matrix elements. In spite of all these theoretical points of dispute, however, the relationship with Bohr, and especially Heisenberg, both of whom behaved toward me in a touchingly kind, nice, caring, and attentive manner, was totally, cloudlessly amiable and cordial."<sup>(486)</sup>

The reports from Copenhagen on the results of the discussions with Schrödinger sounded a little different. For example, Niels Bohr wrote to Ralph Fowler on October 26, 1926: "...The discussions gradually centered themselves on the problems of physical reality of the postulates of atomic theory. We all agreed that a continuity theory [such as Schrödinger's] leads to expectations fundamentally different from those of the usual discontinuity theory [of Born, Heisenberg, Jordan, and Dirac]. Schrödinger himself continued in the hope that the idea of stationary states and

transitions was altogether avoidable, but I think we succeeded at least in convincing him that for the fulfillment of his hope he must be prepared to pay a cost, as regards reformation of fundamental concepts, formidable in comparison with that hitherto contemplated by the supporters of the idea of a continuity theory of atomic phenomena."<sup>(487)</sup> Schrödinger obviously believed that matrix mechanics implied that single stationary states possessed no physical reality, a point of view which Bohr found to be "a confounding of the means and aims of Heisenberg's theory."<sup>(487)</sup> On the other hand, Bohr considered wave mechanics "so wonderfully suited to bring out the true correspondence between the quantum theory and the classical ideas."<sup>(487)</sup> This correspondence was explored by Bohr and his collaborators in the months following Schrödinger's visit to Copenhagen and helped enormously in establishing the physical interpretation of quantum mechanics. The efforts of the Copenhagen physicists on the physical interpretation of quantum mechanics led, in particular, to Heisenberg's uncertainty relations and to Bohr's complementarity view--which became the central parts of the so-called Copenhagen interpretation of quantum mechanics.

### 17.6. The Compton Effect and the Photoelectric Effect

In Section 1 of his paper on the Compton effect, Walter Gordon began by establishing a suitable relativistic wave equation, i.e., Eq. (215).<sup>(476)</sup> In the next Section 2, he showed how to use this equation in order to obtain the emission of radiation from an atomic system. In order to consider the Compton effect (in Section 3), Gordon represented the primary X-radiation by a linearized polarized wave with direction cosines  $n_1$ ,  $n_2$ , and  $n_3$  and the frequency v. The X-rays then create an external potential

$$\Phi_{\alpha} = a_{\alpha} \cos \phi \tag{216}$$

with the phase  $\phi$  given by

$$\phi = \sum_{\alpha} l_{\alpha} x_{\alpha}, \quad \text{where} \begin{cases} l_{k} = \frac{2\pi\nu}{c} n_{k} & \text{for } k = 1, 2, 3\\ l_{4} = i \frac{2\pi\nu}{c} \end{cases}$$
(216a)

These potentials are inserted in Eqs. (215) and yield the wave equation describing the Compton effect, i.e.,

$$\sum_{\alpha} \frac{\partial^2 \psi}{\partial x_{\alpha}} - \frac{4\pi i}{h} \left( \frac{e}{c} \sum_{\alpha} a_{\alpha} \frac{\partial \psi}{\partial x_{\alpha}} \right) \cos \phi - \frac{4\pi^2}{h^2} m^2 c^2 \psi = 0$$
(217)

Gordon solved this equation by making the appropriate Ansatz for  $\psi$ , and determined the frequency of the X-rays shifted by the Compton effect. In particular, he found that the result implied an equation,

$$p_{\alpha} + \pi_{\alpha} = p'_{\alpha} + \pi'_{\alpha} \tag{218}$$

which stated the energy-momentum conservation for the system consisting of the atom (four-momenta  $p_{\alpha}$  and  $p'_{\alpha}$  before and after the impact of the X-radiation) and the radiation (four-momenta of the quanta being  $\pi_{\alpha}$  and  $\pi'_{\alpha}$ , respectively), i.e., just as the old relation of Compton and Debye. Further, the well-known frequency relation followed. Finally, Gordon calculated the intensity *I* of the Compton radiation, obtaining the result

$$I = \sqrt{I_{cl} \cdot I'_{cl}} \tag{219}$$

that is, the quantum-theoretical intensity was equal to the geometrical average of the corresponding classical quantities in the initial  $(I_{cl})$  and the final  $(I'_{cl})$  states. The same result had already been obtained earlier by Gregory Breit on the basis of correspondence considerations<sup>(438)</sup> and by Paul Dirac in his relativistic *q*-number theory.<sup>(430)</sup>

Schrödinger himself approached the wave mechanical treatment of the Compton effect on a far less technical level.<sup>(489)</sup> In pursuing his attempted goal of an intuitive treatment, Schrödinger recalled one of his earlier papers, in which he had investigated the reflection of light waves (of wavelength  $\lambda$ ) from a compression, i.e., a sound wave (of wavelength  $\Lambda$ ); he had then shown that the famous Bragg relation of the classical theory, i.e., the law accounting for the reflection of first-order X-rays from a lattice with lattice constant  $\Lambda$ ,

$$2A\sin\theta = \lambda \tag{220}$$

could be taken over into quantum theory, provided he applied the lightquantum hypothesis to both radiation and sound phenomena.<sup>(490)</sup> The situation in Compton scattering resembled the old light-sound scattering; hence the question arose as to whether an equation of the type of Eq. (220) would also follow from a wave mechanical calculation, and further, if so, whether then the known shift of X-rays when scattered by electrons bound in atoms would result.

Schrödinger proceeded in the most simple manner. He first wrote the wave equation determining the propagation of a free electron in space, i.e.,

$$\Delta \psi - \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} - \frac{4\pi^2 v_0^2}{c^2} \psi = 0$$
 (221)

This wave equation possessed, as the simplest solution, a plane wave,

$$\psi \sim \exp\left\{\frac{2\pi i}{h}\left[hvt - \frac{h\sqrt{v^2 - v_0^2}}{c}\left(\alpha x + \beta y + \gamma z\right)\right]\right\}$$
(222)

where  $\alpha$ ,  $\beta$ ,  $\gamma$  denoted direction cosines ( $\alpha^2 + \beta^2 + \gamma^2 = 1$ ),  $h\nu$  the energy of the moving electron, and  $h\nu_0$  ( $=mc^2$ ) the energy of the electron at rest. According to Schrödinger's discussion in the fourth communication, a  $\psi$ -wave of the type (222) creates a density distribution which is constant in time. If, however, one superposes two such plane waves—the second one having frequency  $\nu'$  and direction cosines  $\alpha'$ ,  $\beta'$ ,  $\gamma'$ —a "wave of electrical density"<sup>(491)</sup> is created which has a structure similar to the sound wave considered by Schrödinger earlier.<sup>(490)</sup> The reflection of a light wave then indeed followed Bragg's law, Eq. (220). One of the immediate consequences was that the energy-momentum four-vectors of the incident and scattered radiation and the corresponding four-vectors of the electron (which is initially bound in the atom and finally leaves it as a free electron) satisfy the Compton–Debye relation, Eq. (218).

A little earlier, before Schrödinger's investigation of the Compton effect was completed, Gregor Wentzel from Leipzig submitted a paper "On the Theory of the Photoelectric Effect" to Zeitschrift für Physik, where it was received on November 19, 1926.<sup>(491)</sup> In this paper, Wentzel opened the path for dealing with the photoelectric effect in wave mechanics. In a second short note, Wentzel completed his treatment of the photoelectric effect in wave mechanics, and included in his calculation the influence of the magnetic field of the incident radiation.<sup>(492)</sup>

### 17.7. Further Successes of Wave Mechanics in the Second Half of 1926

From the middle of the year 1926 onwards, wave mechanics occupied an increasing importance in the physical literature on atomic theory. The number of theoretical physicists using Schrödinger's methods in order to treat a variety of old and new problems grew considerably. Among the contributors to the applications of wave mechanics were physicists, who had for years made a name for themselves in atomic and quantum theory like Peter Debye, Hendrik Kramers, Ralph Kronig, and Fritz Reiche—as well as newcomers like the Dane Øyvind Burrau, the Belgian Charles Manneback, and the Americans J. Robert Oppenheimer and Isidor I. Rabi. The fact that the youngsters also demonstrated their ability to master Schrödinger's methods, so soon after their publication, provided a signal for what later became the triumphant march of wave mechanics.

In a short communication, entitled "Quantum Theory of the Con-

tinuous Absorption Spectrum" and published in the Naturwissenschaften issue of December 24, 1926, (493) Oppenheimer drew attention to his recent work on applying undulatory mechanics "to the hyperbolic orbits of the hydrogen atom" that had been published recently.<sup>(494)</sup> He wrote: "The formulas [obtained] ... provide an estimate of the intensity of the continuous X-ray absorption spectrum. This [estimate] is-I believe-the first experimental check of these parts of the [undulatory] theory."(493) According to the results obtained by Oppenheimer, the absorption of the X-rays begins-the atomic electron being in an orbit described by the quantum numbers n (principal) and k (azimuthal)—at the limit of the corresponding series, assuming there a value proportional to the wavelength of the series limit. Further, for very hard (short-wavelength) X-rays, the absorption coefficient is proportional to the product of a certain power of the wavelength and another power of the effective charge of the atomic nucleus; the calculated numerical values for these power coefficients agreed with the corresponding values derived from the empirical formulas.

Oppenheimer completed the work on his doctoral dissertation under Max Born a few months after his arrival in Göttingen in the fall of 1926. An abridged version of this thesis, entitled "On the Quantum Theory of Continuous Spectra," was published in *Zeitschrift für Physik* early in 1927.<sup>(495)</sup> Oppenheimer organized the material of this thesis in three parts. 1. General Theory; 2. Application to the Two-Body Problem; 3. Physical Results. In Part 1, he displayed the solution of the (time-independent) Schrödinger equation of a general atomic system which possesses a discrete and continuous energy spectrum. In part 2, Oppenheimer applied the general theory to the class of atoms consisting of a heavy nucleus of mass *M* and electric charge *Ze*, which attracts an electron with a distorted (Coulomb) potential

$$V = -\frac{Ze^2}{r} - \frac{b}{r^2}$$
(223)

where b denotes a small constant. He solved the wave equation of this system in the standard manner. In Part 3, Oppenheimer applied his results to the simplest case of the hydrogen atom, where the second term—with b=0—in Eq. (223) drops out. Thus, he calculated the properties of the continuous absorption spectra which join the discrete series spectra of atomic hydrogen on the short wavelength side. In particular, he found an explicit formula for the coefficient of absorption  $\alpha$ , expressed as a function of the wavelength  $\lambda$  of the absorbed radiation. Oppenheimer also used his theory to deal with two other physical problems: namely, the photoelectric effect and *Bremsstrahlung*.

The Belgian Charles Manneback, then working with Peter Debye at the E.T.H. in Zurich, completed a paper on July 17, 1926 on "The Dielectric Constant of Diatomic Dipole Gases According to Wave Mechanics" and submitted it to Physikalische Zeitschrift. (496) This problem was a rather fashionable one in those days, besides being of considerable interest for Manneback's host Debye. For instance, Lucy Mensing and Wolfgang Pauli had very recently-in June 1926-obtained a result with the help of matrix mechanical methods which appeared to be more satisfactory than the result based on the old quantum theory, insofar as it passed over into the classical solution of Debye<sup>(17)</sup> in the limit of high temperatures.<sup>(497)</sup> Manneback formulated and solved the problem in the context of wave mechanics, and concluded: "One arrives, in Schrödinger's mechanics, at exactly the same results as in the mechanics of Heisenberg and Born: the dielectric constant of an ideal diatomic gas composed of rigid molecules ... approaches the value given by the theory of Langevin and Debye at high temperatures."<sup>(498)</sup>

A little more than a month after Manneback had submitted his paper on the rigid diatomic molecule, Fritz Reiche from Breslau sent a paper, entitled "The Quantization of the Symmetrical Top According to Schrödinger's Undulatory Mechanics," to Zeitschrift für Physik.<sup>(499)</sup> The symmetrical top represented a generalization of the rigid rotator that had been solved by Schrödinger in his second communication and had played a role in Manneback's work: instead of one moment of inertia, it possessed three such moments, A, B, and C, two of which were identical, i.e., A = B. Reiche established the wave equation for his problem in the standard way, which was given by Schrödinger in his paper on the equivalence of the two theories.<sup>(500)</sup> In the case of the free symmetrical top, Reiche obtained the discrete energy values

$$E = \frac{h}{8\pi^2} \left[ \frac{j(j+1)}{A} + \left(\frac{1}{c} - \frac{1}{A}\right) \tau^2 \right]$$
(224)

where  $\tau$  assumed positive and negative integral values, and *j* positive integral values larger than or equal to the absolute value of  $\tau$ . In the case of a symmetrical top—with whose axis an electric dipole moment was connected—Reiche investigated the motion in an external homogeneous electric field of strength *F* parallel to the *z*-axis (so that the potential energy  $V = \mu F \cos \theta$ ), and obtained the additional energy term

$$\delta E^{(1)} = -\mu F \frac{|\tau| \cdot |\tau'|}{j(j+1)}$$
(225)

where  $\tau$ ,  $\tau'$ , and *j* assume integral values such that

$$0 \leq |\tau| \leq j \text{ and } 0 \leq |\tau'| \leq j$$
 (225a)

and  $\mu$  is the electric moment of the permanent dipole (associated with each molecule) and  $\theta$  the angle between the axis of the dipole moment and the vector of the electric field.

As a special application of his result, Eq. (224), Reiche tried to explain the problem of the rotational heats of hydrogen. In a second paper, bearing the same title and submitted in late November 1926 (again to *Zeitschrift für Physik*), Reiche and Rademacher studied the problem of intensities of radiation that can be emitted by a symmetrical top.<sup>(501)</sup> For that purpose, they calculated the matrices of the electric moment of the system in a coordinate system fixed in space and found, after detailed calculations, results which agreed with those obtained in the spring of 1926 by David M. Dennison.<sup>(502)</sup> They further noticed that their intensity formulas derived for a spinning top in the presence of a weak perturbing electric field agreed fully with those of Lucy Mensing, in the special case which the latter had evaluated by using matrix methods.<sup>(380)</sup>

In November 1926, Ralph de Laer Kronig and Isidor I. Rabi from Columbia University, New York, also submitted their paper on "The Symmetrical Top in the Undulatory Mechanics" to the *Physical Review*.<sup>(503)</sup> Their approach fully agreed with that of Reiche and Rademacher. Kronig and Rabi noticed the identity of their result [Eq. (224), same as Reiche's] with Dennison's, and further calculated explicitly the matrix elements for the *z*-component of the transition amplitude. The results were again identical with those obtained by matrix methods. The American authors performed their calculations completely on their own, unaware of the European competition.

In a further paper on "Dielectric Constant and Stark Effect of Polyatomic Dipole Gases with Symmetrical Molecules According to Wave mechanics,"<sup>(504)</sup> Manneback explicitly displayed the establishment of the wave equation of the symmetrical top and obtained the energy eigenvalues, Eq. (224), in the case of zero potential, as well as the corrections due to a perturbing electric field. In the rotation-free case, j = 0, the correction  $\delta E^{(1)}$ , Eq. (225), disappears, and Manneback computed the quadratic correction to be

$$\delta E^{(2)} = -\frac{1}{6} \frac{(\mu F)^2}{(h^2/8\pi^2 A)}$$
(226)

Manneback's wave mechanical treatment of the symmetrical top was independent of that of Kronig and Rabi. Hence, all three wave mechanical treatments of the symmetrical top—those of Reiche, Kronig and Rabi, and Manneback—were arrived at independently. They confirmed the results obtained earlier on the basis of matrix mechanics.

Another application of wave mechanical methods, however, probed entirely new ground. In the summer of 1926, Waldemar Alexandrow in Zurich undertook to solve the problem of the hydrogen molecule-ion in the framework of wave mechanics, a problem which Wolfgang Pauli<sup>(505)</sup> and K. F. Niessen<sup>(506)</sup> had worked on in their respective doctoral theses according to the Bohr–Sommerfeld theory. In a letter, dated June 11, 1926, Pauli reported to Wentzel: "In Copenhagen, there is a gentleman who occupies himself with the calculation of H<sub>2</sub><sup>+</sup> [hydrogen molecule-ion], according to Schrödinger['s wave mechanics]." It took the gentleman in question, Øyvind Burrau, some time to handle the problem.

Alexandrow started from Schrödinger's fundamental equation and, after introducing elliptical coordinates, made use of the *Ansatz* for the separation of variables for the wave function, obtaining solutions for the resulting second-order equations. For the ionization potential of the hydrogen atom, he obtained the value of 13.5 volts, which seemed to be in agreement with observation—notably that of the ionization potential of the hydrogen molecule.

After a close scrutiny of Alexandrow's paper, Heisenberg wrote to Pauli: "The work of Alexandrow... [is] naturally totally wrong."<sup>(507)</sup> He reported further: "Here [Friedrich] Hund has ceded the  $H_2^+$  to Mr. Burrau, and the latter has now really straightened out the problem finally.... Burrau obtains, as one should, solutions whose Schrödinger functions don't have any zeros; he computes the energy as a function of the distance of the nuclei and connects [the energy], on the one hand, to [that of the] He<sub>1s</sub> state, and, on the other hand, to that of the H<sub>1s</sub> state. By the way, the  $\psi$ -function is symmetrical with respect to the nuclei. If one adds [the potential energy of] the repulsion to the energy, then one gets a nice minimum [of the energy] at [a distance of the nuclei]  $r \approx 3a_H$  (that is, about half the distance that you found at that time); and the energy is 15.7 volts, which is accurate enough in any case. About this [problem], one can therefore calm down."<sup>(507)</sup>

Burrau's paper on the "Calculation of the Energy Value of the Hydrogen Molecule-Ion  $(H_2^+)$  in the Ground State" was ready for publication, after much delay, on March 19, 1927.<sup>(508)</sup> Burrau's work, apart from minor later improvements, finished the problem. The ground state energy of the hydrogen molecule-ion, corrected slightly by taking into account the zero-point energy  $\frac{1}{2}hv$  of the oscillations of the nulcei, was finally found to be

$$-E_{\rm tot} = 16.22 \text{ volts}$$
 (227)

## 17.8. Schrödinger's Rising Fame: Visit to America and Call to Berlin Professorship

Although the final success of the hydrogen molecule-ion calculation —the second crucial test of a complicated calculation of atomic energy states after Heisenberg's solution of the helium problem—had not been fully secured by late 1926, the experts were confident enough at that time that more or less *all* the problems of atomic structure could be handled by means of wave mechanical methods. This situation must certainly have pleased Schrödinger, as much as it excited and astonished the community of physicists. It did not mean, however, that no questions remained to be answered in the theory, and Schrödinger himself was the first person to be aware of the unresolved difficulties. Especially, he was deeply concerned about the fundamental problems connected with the interpretation of the wave function and the relation between the wave mechanical quantities and those of (classical) electrodynamics.

During the last few months of 1926 Schrödinger was hindered from continuing to consider the problem of interpretation in detail due to the preparations for his extended visit to America. In the United States, wave mechanics had increasingly attracted the attention of physicists from the West to the East Coast. The principal invitation to Schrödinger came from Charles E. Mendenhall to deliver an extended series of lectures at the University of Wisconsin in Madison. Schrödinger finished his lecturing duties at the University of Zurich and left the city on December 18, 1926, together with his wife, travelling via Basel and Paris to Le Havre, from where he sailed on the French liner De Grasse for New York. In New York, Karl Herzfeld and Friedrich Paneth, two old acquaintances from Vienna, welcomed the Schrödingers, and helped them through customs and in finding accommodations. After an extended stay in New York, they travelled westwards and arrived on January 2 in Madison, where Schrödinger assumed his duties. During his stay there, a meeting on quantum theory was held at the University of Wisconsin (on January 22, 1927); this provided Schrödinger the opportunity to meet several American physicists active in this field: for example, the experimentalist George Eric MacDonnell Jauncey-the X-ray and Compton scattering specialist from St. Louis-and the young theoreticians John H. Van Vleck (from Minneapolis) and Frank C. Hoyt (from Chicago).

Schrödinger's presence in America was not restricted to Madison, Wisconsin. He received and accepted invitations at neighboring places like Minneapolis and Chicago. On February 10, 1927, when the lecture course in Wisconsin was completed, the Schrödingers travelled further west to California, first to Pasadena, where they stayed two weeks. At the California Institute of Technology, a series of lectures on wave mechanics had been arranged, which Schrödinger had the pleasure and privilege of delivering together with the venerated senior physicist Hendrik Lorentz, who had been invited at the same time.<sup>(509)</sup> In these lectures on wave mechanics at Caltech, Lorentz took over the parts on the foundations of the theory, leaving Schrödinger free to elaborate on special problems and applications. The audience was rather large: about sixty physicists participated regularly. Paul Epstein, the theoretician at Caltech, not only showed a professional interest in wave mechanics, but also took the visitors sightseeing, e.g., to Mount Wilson.

From California, the Schrödingers went back to Chicago (March 7, 1927); Ann Arbor, Michigan; Boston and Cambridge, Massachusetts (Harvard University); then Baltimore (March 21), where Schrödinger met the spectroscopists Robert W. Wood and Alfred L. Loomis. Altogether he delivered 57 lectures—not all of them on topics of atomic theory—the last one at Columbia University, New York, before he returned home. On April 10, 1927, Schrödinger was back in Zurich.

The American tour was a strenuous enterprise, although Schrödinger enjoyed it more the longer it lasted. It added substantially to his reputation as a physicist outside Europe, and even more, it helped to propagate wave mechanics. Mendenhall offered him a permanent position at the University of Wisconsin, indeed an honorable offer, which, however, Schrödinger did not accept. One of the reasons was that, before he left Europe, Max Planck had informed him of a most exciting prospect: the possibility that he might be called (*berufen*) to occupy the chair of theoretical physics at the University of Berlin as Planck's successor.

Arnold Sommerfeld was a prime candidate for the chair of theoretical physics at the University of Berlin. Although his negotiations with the Prussian Ministry of Education went on for some time, he ultimately declined in July 1927. The call then went to Schrödinger. He spent quite some time dealing with the Prussian authorities, and at the same time entered into active negotiations with Zurich; he soon realized that the authorities at the University of Zurich and the E.T.H. were more interested in increasing his duties than in granting him privileges. On September 3, 1927, he wrote to Wien: "Now the decision has been made. I am certainly able to say, now that it has been decided, that I shall really go to Berlin with pleasure. Every imaginable courtesy has been granted to me there; I could see that people really want to get me, which is indeed always a pleasant feeling."<sup>(510)</sup> In the autumn of 1927, Schrödinger went to Berlin and joined the university as professor of theoretical physics; his closest colleagues were Max von Laue and Albert Einstein, who esteemed his work highly and had helped in bringing him to Berlin, although the driving power had been Max Planck, the man whom he succeeded.

Schrödinger's stay in Berlin from 1927 to 1933 was very happy. As Annemarie Schrödinger recalled: "Berlin [had] the most wonderful and absolutely unique atmosphere for all scientists.... The theatre was at its height, the music was at its height, and science with all the scientific institutes [and] industry. And the most famous *Kolloquium*.... It was the most famous colloquium I think ever held: Lise Meitner, Einstein, Planck, Nernst, Haber, [Gustav] Hertz, [Peter] Pringsheim—a terrific lot [of famous] people.... There were lots of friends who came together, not [only] on a special day; it was absolutely a very nice social life. My husband liked it very much indeed."<sup>(511)</sup>

Schrödinger, the new member of the distinguished circle of physicists, arrived in Berlin with a fresh laurel wreath wrapped around his theory. In recent months, the results of two independent experiments had been published, one carried out by Clinton Joseph Davisson and Lester Halbert Germer in America,<sup>(512)</sup> the other by George Paget Thomson and Alexander Reid in Scotland,<sup>(513)</sup> which proved the wave nature of electrons, i.e., the reality of matter waves, the basis of wave mechanics. Schrödinger was very happy about the experimental confirmation of de Broglie's conception of matter waves, but his colleagues in Berlin considered wave mechanics as the real theoretical fulfillment of the idea of matter waves. They received him cordially with all honors, and made him feel like a preferred member of their community by electing him (in 1929) as a member of the Prussian Academy of Sciences.

Mrs. Schrödinger recalled: "When we came to Berlin we thought: 'Well, we will stay in Berlin for a good while.' We couldn't have thought that we'd have to leave Berlin."<sup>(511)</sup> Still, the necessity came in 1933, after the German government was taken over by the Nazis. Shocked by the new politics in general, and by the dismissal of the Jewish scientists from their positions in particular, Schrödinger resigned voluntarily from his Berlin professorship and left Germany to assume a position at Oxford University in November 1933. Soon after arriving in Oxford, Erwin Schrödinger received the news that he was to share the Nobel prize in physics for the year 1933 with Paul Adrien Maurice Dirac, while Werner Heisenberg was awarded the prize for the year 1932. Then a new chapter in Schrödinger's life began.

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## Schrödinger and the Rise of Wave Mechanics

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## Schrödinger and the Rise of Wave Mechanics

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- 430. P. A. M. Dirac, Relativity Quantum Mechanics with an Application to Compton Scattering, Proc. R. Soc. London A 111, 405-423 (1926). Dirac noted in this paper that some difficulties arise between the "quantum energy" E and the quantum mechanical Hamiltonian, because the new variable E ought to commute with, say, the position variable, whereas the Hamiltonian does not do so.
- 431. This was an old question in statistical mechanics, which led in the early 1920s to a great discussion between two groups, with Einstein and Planck advocating the indistinguishability of particles (see, e.g., M. Planck, Ref. 210) and Ehrenfest and Schrödinger raising objections (e.g., E. Schrödinger, Ref. 181).
- 432. E. Fermi presented a short note, Sulla quantizzazione del gas perfetto monoatomico, *Rend. R. Accad. Lincei* 3, 145–149 (1926), on February 7, 1926, and an extended version, Zur Quantelung des idealen einatomigen Gases, Z. Phys. 36, 902–912 (1926), was received on March 26, 1926. Fermi wrote to Dirac on September 1926, drawing his attention to his own earlier work.
- 433. P. A. M. Dirac, in Conversations with J. Mehra, June 1968 at Trieste, Italy; also AHQP Interview with Dirac.
- 434. E. Schrödinger, Ref. 244, p. 372; English translation, p. 9.

- 435. E. Schrödinger, Ref. 256, pp. 489-514.
- 436. E. Schrödinger, Ref. 256, p. 506; English translation, p. 25.
- 437. E. Schrödinger, Ref. 256, p. 508; English translation, p. 26.
- 438. Letter from W. Wien to E. Schrödinger, May 13, 1926.
- 439. E. Schrödinger, Ref. 349, p. 735, footnote 2; English translation, p. 46, footnote 1.
- 440. E. Schrödinger, Ref. 349, p. 751.
- 441. Schrödinger demonstrated this point by observing that one can obtain in matrix mechanics all "moments" of the product function  $u_i(x) u_k(x)$ , especially  $u_i^2(x)$ , from suitable matrix elements; thus the function  $u_i(x)$  follows. (We may note here that Schrödinger so far treated eigenfunctions more or less as real functions.)
- 442. E. Schrödinger, Ref. 349, p. 752.
- 443. E. Schrödinger, Ref. 349, p. 753; English translation, p. 59. Schrödinger's claim with respect to the possibility of treating collision processes in wave mechanics was substantiated a few months later by the work of Max Born, as we have reported earlier.
- 444. Letter from E. Schrödinger to W. Wien, June 18, 1926.
- 445. Letter from E. Wigner to J. Mehra, November 20, 1985.
- 446. E. Schrödinger, Quantisierung als Eigenwertproblem. (Vierte Mitteilung), Ann. Phys. 81, 109-139 (1926), p. 109; in Collected Papers on Wave Mechanics, pp. 102-123, p. 102.
- 447. E. Schrödinger, Ref. 446, p. 110; English translation, p. 103.
- 448. E. Schrödinger, Ref. 446, p. 110; English translation, p. 103.
- 449. R. Courant and D. Hilbert, Ref. 313, Chapter V, Section 8.
- 450. This decomposition is by no means trivial mathematically; however, it can be shown to be valid in the case mentioned. Thus Eq. (398) leads to two equations,

$$\left(\varDelta - \frac{8\pi^2}{h^2} V + \frac{8\pi^2}{h^2} E\right)\psi = 0$$

and

$$\left(\varDelta - \frac{8\pi^2}{h^2} V - \frac{8\pi^2}{h^2} E\right) \psi = 0$$

of which the second one provides physically no new information (as the parameter E is simply replaced by -E).

- 451. P. A. M. Dirac, Ref. 428, pp. 674-676.
- 452. P. A. M. Dirac, The Quantum Theory of Emission and Absorption of Radiation, Proc. R. Soc. London A 114, 243-265 (1927); The Quantum Theory of Dispersion, Proc. R. Soc. London A 114, 610-624 (1927).
- 453. Letter from W. Wien to E. Schrödinger, June 23, 1926.
- 454. See the announcement in Verh. Dtsch. Phys. Ges. 7, 36 (1926). Walther Nernst chaired the meeting.
- 455. The meeting was chaired by the astrophysicist Robert Emden. [See Verh. Dtsch. Phys. Ges. 7, 38 (1926).]
- 456. E. Schrödinger, An Undulatory Theory of the Mechanics of Atoms and Molecules, *Phys. Rev.* 28, 1049–1070 (1926).
- 457. E. Schrödinger, Ref. 456, p. 1049.
- 458. E. Schrödinger, Ref. 456, p. 1050.
- 459. E. Schrödinger, Ref. 456, p. 1070.
- 460. E. Schrödinger, Ref. 446, p. 139; English translation, p. 123.
- 461. Letter from A. Einstein to A. Sommerfeld, August 21, 1926.
- 462. W. Heisenberg, Gesammelte Werke/Collected Works, Series C/Volume IV: Biographisches und Kernphysik, (R. Piper Verlag, Munich, Zurich, 0000), pp. 26-27.

## Schrödinger and the Rise of Wave Mechanics

- 463. Letter from A. Sommerfeld to W. Pauli, July 26, 1926.
- 464. E. Schrödinger, Ref. 446, pp. 133-134; English translation, p. 119.
- 465. Letter from W. Pauli to P. Jordan, Ref. 363, Eq. (3).
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- 467. T. Kaluza, Zum Unitätsproblem de Physik, Sitzber. Preuss. Akad. Wiss. (Berlin), 966-972 (1921).
- 468. O. Klein, Ref. 466, p. 895.
- 469. The nonrelativistic form of the Schrödinger equation for hydrogen results, if one puts  $hv = mc^2 + E$  and  $|E| \ll mc^2$ .
- 470. V. Fock, Zur Schrödingerschen Wellenmechanik, Z. Phys. 38, 242-250 (1926).
- 471. V. Fock, Über die invariante Form der Wellen- und der Bawegungsgleichungen für einen geladenen Massenpunkt, Z. Phys. 39, 226–232 (1926).
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- 473. Th. De Donder, Application de la quantification de la Gravifique einsteinienne, *Compt. Rend. (Paris)* 183, 594-595 (1926).
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- 479. Letter from W. Heisenberg to W. Pauli, July 28, 1926.
- 480. Letter from N. Bohr to E. Schrödinger, September 11, 1926.
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- 483. Telegram from E. Schrödinger to N. Bohr, September 27, 1926.
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- 485. See J. Mehra and H. Rechenberg, Ref. 481, p. 823, and footnote 295.
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