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ON THE HISTORY OF EARLY WAVE MECHANICS

WITH SPECIAL EMPHASIS ON THE ROLE OF RELATIVITY

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INTRODUCTION

The years 1925 and 1926 are truly the *anni mirabili* of quantum physics. In a very short span of time, covering only about ten months, the crisis of the old quantum theory was resolved and a completely new understanding of micro-physical phenomena had been architectured. The chief architects were, of course, Heisenberg and Schrödinger, and the buildings they raised were matrix mechanics and wave mechanics.

If quantum mechanics represented a thorough conceptual break with classical and semi-classical ideas, so did the theory of relativity, often mentioned together with quantum mechanics as constituting the 'new physical world picture'. At the time when quantum mechanics developed, the theory of relativity had been an integrated and fully accepted part of physical theory for many years, and had been successfully applied to numerous problems in micro- as well as macrophysics. In 1925, a physical theory could only be considered as completely satisfactory if it was in accorcance with the principle of relativity. Yet, when matrix and wave mechanics entered the scene of science, it was in strictly non-relativistic forms.

In the present work, the role of relativity in the creation of the new mechanics, particularly wave mechanics, is subjected to a detailed examination. The general result is that, contrary to what should be expected from the classical publications themselves, wave mechanics was thoroughly mixed up with relativity. Historically, Schrödinger's mechanics *is* a relativistic theory. Although it might have been found without considering relativity (which is the standard approach taken in textbooks), Schrödinger's route to wave mechanics is hardly imaginable on a non-relativistic basis. Apart from relativity, the hydrogen spectrum may be taken as another crucial element in the creation of wave mechanics, I suggest. In the development of matrix

and wave mechanics, the two prime test cases were the anharmonic oscillator (for matrix mechanics) and the hydrogen atom (particularly for wave mechanics).
For Schrödinger, the hydrogen case was furthermore tightly connected with the question of relativity.

Schrödinger's celebrated discovery of wave mechanics has been subject to historical investigations at several occasions and by several authors, to be mentioned below. There are, however, serious lacunae in the historical writings on the subject, hitherto published. Many of these lacunae are, I think, due to a lack of realizing the crucial role of relativity in the creation of wave mechanics.

Also, what is perhaps the most important source material as regards the formation of wave mechanics, Schrödinger's research notebooks, has never been duly incorporated in the historical investigations of wave mechanics. In this work, I try to take full advantage of Schrödinger's notebooks as well as of other unpublished material.

The aim of the present text is not to give a comprehensive or complete history of the genesis of wave mechanics. Important contributions to this end have already been supplied by historians of science, and there is no need duplicating their research. Rather, my aim is to present a cross-section of the earliest wave mechanics and its debts to relativity. In this context, I have paid particular attention to the work of Oskar Klein, largely neglected by historians of quantum physics.

The story of the interplay between quantum mechanics and relativity might, of course, be continued also after the summer of 1926, which is largely where I stop. In another paper, focusing on Dirac's creation of a truly relativistic wave mechanics in 1928, I have dealt with elements of the development of relativity quantum mechanics after 1926. In a sense, this other paper is a continuation of the story here told.

§ 1. ELECTRONS, QUANTA AND RELATIVITY IN DE BROGLIE'S THEORY

The main sources to Erwin Schrödinger's wave mechanics were the works of Albert Einstein and Louis de Broglie. Indeed, a short time before Schrödinger engaged in the development of his undulatory theory, he had stated his programme "als ernst machen mit der de Broglie-Einsteinschen Undulationstheorie."[1] Einstein's contributions to the emergence of wave mechanics were indirect, but profound. For one thing, the theory of relativity played a very important role in de Broglie's as well as in Schrödinger's thinking about waves and particles. For another thing, Einstein's contributions to quantum statistical theory were highly influential to Schrödinger's route to wave mechanics. And for a third thing, it was primarily as a result of Einstein's endorsement of de Broglie's ideas, that they became accepted, and eventually transformed by Schrödinger.

The immediate predecessor of wave mechanics was, however, not Einstein, but de Broglie. For the benefit of the further discussion of Schrödinger's theory, it may therefore be convenient to recall the essentials of de Broglie's theory. Since this theory has been treated detailedly by historians of science,[2] I shall suffice to present only some of de Broglie's main results, of particular relevance to our subject. Although most of de Broglie's results were published already in 1922-1923, in several smaller articles, the by far most complete and mature form of the theory appeared in late 1924, in de Broglie's doctoral dissertation.[3] It was also this *These* which became of particular importance to wave mechanics, such as created by Schrödinger. In the following review, I shall rely on this work, and particularly on its first half, the one which deals with so-called matter waves.

In the very beginning of this thesis, de Broglie defined his programme to answer the question of "quelle forme nous pouvons faire intervenir les quanta dans la Dynamique de la Relativité."[4] How could, de Broglie asked, a portion of energy be conceived, if not associated a certain frequency? Attempting to bridge quantum theory and relativity, de Broglie simply proposed to combine the two Einsteinian 1905 formulae for the energy of photons and matter, respectively. That is,

$$h\nu_o = m_o c^2 \tag{1.1}$$

This daring and straight-forward combination of quantum theory and relativity, by de Broglie termed "une grande loi de la Nature", was made the foundation of de Broglie's dualistic theory.

If the particle of proper mass m_o moves with velocity β (= v/c), the natural generalization of (1.1) is

$$h\nu = mc^2 = \frac{m_o c^2}{\sqrt{1-\beta^2}} \tag{1.2}$$

due to relativistic mass-variability. But this result, de Broglie emphasized, is contradictory to the one got from the use of relativistic time-dilation. According to the Lorentz transformation, the frequency decreases by the factor $\sqrt{1-\beta^2}$ for a moving particle, so that a fixed observer should find the frequency

$$\nu_1 = \nu_0\sqrt{1-\beta^2} = \frac{m_o c^2}{h}\sqrt{1-\beta^2} \tag{1.3}$$

This disagreement was formally resolved by assigning ν and ν_1 to two different kinds of hypothetical vibrations. While ν_1 is the frequency of the internal periodic phenomenon of the particle, ν was assigned to a travelling wave, supposed to accompany the particle and being in phase with the internal vibration. This wave was called a *phase wave*, and de Broglie proved that its velocity is given by

$$V = \frac{c}{\beta} = \frac{c^2}{v} \tag{1.4}$$

Being larger than the velocity of light, V cannot refer to a physical transport of energy. The physical significant velocity is the group velocity, U, which in general relates to V by Lord Rayleigh's formula

$$\frac{1}{U} = \frac{d}{d\nu}\left(\frac{\nu}{V}\right) \tag{1.5}$$

De Broglie easily proved, by introducing (1.2) into (1.5), that the group velocity of the phase wave equals the velocity of the moving particle, i.e. that

$$U = c\beta = v \tag{1.6}$$

In his further attempts to link together quantum theory and relativity, de Broglie made use of an interesting extension of the principles of least action, known from optics and mechanics. "Guidé par l'idée d'une identité profonde du principe de la moindre action et de celui de Fermat," de Broglie explained, "j'ai été conduit dès le début de mes recherches sur ce sujet *à admettre* que pour une valeur donnée de l'énergie totale du mobile et par suite de la fréquence de son onde de phase, les trajectoires dynamiquement possibles de l'un coincidaient aves les rayons possibles de l'autre."[5] For the mechanical motion of a particle, de Broglie departed from Hamilton's principle of least action, which he transformed to the following, generalized form

$$\delta\int\sum_{i=1}^{4} J_i dx^i = 0 \tag{1.7}$$

valid for a relativistic particle moving in an electromagnetic field. In (1.7), J_i are the covariant components of a "vecteur d'Univers", which is in fact a generalized four-momentum:

$$\left.\begin{aligned} -\vec{J} &= \vec{p} + e\vec{A} \\ J_4 &= \frac{E}{c} + \frac{e}{c}\varphi \end{aligned}\right\} \tag{1.8}$$

with $\vec{A}$ and φ being the electromagnetic potentials and $\vec{p}$ the mechanical momentum $m_o\vec{v}(1 - \beta^2)^{-\frac{1}{2}}$. The contravariant components dx^i in (1.7) are equal to $(d\vec{r}, cdt)$.

The propagation of waves, on the other hand, is determined by Fermat's principle in geometrical optics, and de Broglie showed that it might be linked to Hamilton's (or Maupertuis') mechanical variational principle in a highly suggestive way. For this purpose, de Broglie introduced another four-dimensional world vector, a "vecteur Onde d'Univers," O_i. It was defined by

$$O_i = (-\vec{k}, \frac{\nu}{c}) \tag{1.9}$$

where $\vec{k}$ is the wave number vector, directed along the rays and with the value $|\vec{k}| = {}^1/\lambda = {}^\nu/V$. The phase waves were now shown to be governed by the variational principle

$$\delta\int\sum_{i=1}^{4} O_i dx^i = 0 \tag{1.10}$$

The connection between de Broglie's generalized variational principles and the classical principles of Maupertuis and Fermat may be seen as follows: If $\vec{O}$ is inserted in (1.10), the result is

$$\delta\int\vec{k}\cdot d\vec{r} = \delta\int\frac{\nu}{V}\,ds = o$$

which is Fermat's principle. Similarly, the first three components of (1.7) yield (excluding electromagnetic terms)

$$\delta\int\vec{p}\cdot d\vec{r} = o$$

which is Maupertuis' principle. By virtue of (1.2) and (1.4) Fermat's principle may also be written

$$\delta\int\frac{m_o c\beta}{\sqrt{1-\beta^2}}\,ds = \delta\int p\,ds = o$$

which is again Maupertuis' principle.

The real progress in de Broglie's use of the variational principles was his comparison between (1.7) and (1.10), the one relating to material aspects, the other to wave aspects. In terms of the world vectors, the usual quantum condition $E=h\nu$ may be written as $J_4=hO_4$, and de Broglie suggested that the proportionality also held for the other three components, i.e.

$$J_i = hO_i \quad (i = 1.2.3.4) \tag{1.11}$$

In this way Fermat's principle for the phase wave becomes identical to Maupertuis' principle for the material particle. De Broglie's extension of the quantum law, he admitted, was "un peu hypothétique", but he regarded its "accord profond avec l'esprit de la théorie de la Relativité" as a highly qualifying feature.[6] The novelty in (1.11) is the relation

$$\vec{p} = h\vec{k} \qquad (1.12)$$

or

$$\lambda = \frac{h}{p} = \frac{h\sqrt{1-\beta^2}}{m_0 \beta c} \qquad (1.13)$$

which is often known as 'de Broglie's formula'. In fact, neither this formula nor the accompanying $E=h\nu$ were in themselves de Broglie's discoveries. They had both been found years ago by Einstein.[7] But de Broglie's interpretation was new and unorthodox: while Einstein's equations referred to light quanta only, de Broglie claimed their validity also for material particles, in this way establishing the wanted symmetry between light and matter.

It is sometimes stated that de Broglie did only consider free particles and did not apply his ideas to bound electrons[8] (and, the point is, he was therefore not led to a proper wave mechanics of the atom). This is not quite true. In his thesis, de Broglie applied his ideas of matter waves to the Bohr hydrogen atom, for which he wrote the frequency of the electron's phase wave as

$$h\nu = \frac{m_0 c^2}{\sqrt{1-\beta^2}} + e\varphi \qquad (1.14)$$

where $\varphi = -\frac{e}{r}$. The phase velocity was found to depend on the distance from the nucleus in accordance with

$$V = \frac{c}{\beta} \cdot \frac{E}{E - e\varphi}$$

However, de Broglie was never led to set up a wave equation for the wave in question. Indeed, this was the main difference between de Broglie and Schrödinger.[9]

De Broglie also applied the new viewpoint to propose a wave interpretation of the Sommerfeld-Wilson quantization conditions for the stationary states of an atom. According to these conditions, the stationary states are determined by

$$\int pdq = nh \quad (n = 0,1,2,\ldots) \qquad (1.15)$$

where the integration is taken over a complete cycle and where p and q denote pairs of conjugate momenta-coordinates. In de Broglie's picture of the atom, the path of an electron is identical to the ray of its phase wave. For a stationary state the path must then contain a whole number of waves, $n\lambda = s$; or, in the general case

$$\int \frac{1}{\lambda}\, ds = n \qquad (1.16)$$

But according to the previous results (eq.(1.11)) this equals the phase integral $\int pds$ divided with h. In this way (1.15) is derived as a resonance condition for the phase wave. "Ce beau résultat dont la démonstration est si immédiate quand on a admis les idées du précédent chapitre est la meilleure justification que nous puissions donner de notre manière d'attaquer le problème des quanta."[10]

As is abundantly clear from this review of a part of de Broglie's theory, it was throughout a *relativistic* theory. In its foundation and in its entire spirit, the theory was based on relativity in every detail, a fact repeatedly stressed by de Broglie, then as later.[11] De Broglie thought in 1924 that he had created a fully relativistic quantum theory. Indeed, even if we may extract the non-relativistic approximations of de Broglie's theory, such a thing as a non-relativistic de Broglie theory cannot be imagined.[12]

The second half of the *Thèse* dealt with light quanta and statistical gas theory. We shall not be concerned with this part, even if it was most effective in transferring de Broglie's ideas to Einstein and to Schrödinger. Also in de Broglie's quantum statistics of gases, relativity played a profound role. Many years later, de Broglie stated: "Sans les idées de la relativité et, en particulier, sans la loi relativiste de composition des vitesses, et les formules de la dynamique correspondante, il serait impossible de comprendre les propriétés de lumière."[13]

In regard of the close congruence between de Broglie's and Schrödinger's works, one may ask why de Broglie did not himself develop his theory into a proper wave mechanics, including a wave equation. From a formal point of view, this may seem to have been an obvious possibility since most of the material of which Schrödinger formed his wave mechanics were already contained in de Broglie's theory. This holds not only for the basic conception of particles' wave nature, but also for the methods applied by Schrödinger in his derivation of the wave equation. The role of group velocity, the use of variational principles and the optical-mechanical analogy were all highligthed by de Broglie.

Kubli[14] has called attention to two kinds of reasons why de Broglie's theory remained a rather hypothetical approach and was not, by de Broglie, developed into a proper wave mechanics. For one thing, a number of 'external' reasons made de Broglie less suited to follow a route á la Schrödinger. De Broglie's mathematical and physical knowledge was, for instance, incomplete on some central issues, due to a generally low standard of French science education, especially as regards mathematical analysis. In 1914, de Broglie was thus not acquainted with the theory of eigenvalue problems. Also, de Broglie was isolated from the mainstream of theoretical physics taking place in particular in Germany. In contrast, Schrödinger's professional background and mathematical training was first class and particularly well suited for his coming work in wave mechanics.[15]

But even if de Broglie was, by these and other reasons, badly equipped to develop his ideas into a wave mechanics, they do not explain why he didn't attempt to put up a wave equation such as can very easily be done from de Broglie's formulae (see § 8). For this question we must turn to 'internal' reasons, i.e. the differences between de Broglie's and Schrödinger's research programmes. It was de Broglie's aim, then as later, to establish a purely dualistic theory of waves and particles. For this purpose he constructed his *phase* waves which he imagines as progressing waves associated mainly to free particles. Schrödinger's ambitions, on the contrary, were to substitute waves for material particles, which he represented as wave packets. Schrödinger's main concern was, furthermore, with the amplitudes of the waves, not with their phases. His waves were not progressive, but standing waves: "Der Hauptunterschied ist, dass de Broglie an fortschreitende Wellen denkt, während wir, wenn wir unseren Formeln die Schwingungsvorstellung unterlegen, auf stehenden Eigenschwingungen geführt werden."[16] The Schrödinger equation is an amplitude equation, corresponding to the one governing standing waves in a vibrating string. It is formally, but not conceptually, within the range of de Broglie's framework.

One should realize that there is an unbridgeable gap between the formal setting up of equations and the conceptual creation of a theory which rests on these equations. Formulae are not theories. This rather obvious point may be relevant to various speculations about how wave mechanics *could* have been created. Friedrich Hund has argued that de Broglie's ideas of matter waves could, and should(?), have been the natural outcome of Einstein's theories from 1905 and 1917: "Einstein selbst hätte den

Dualismus auf die Materie ausdehnen und seine eigene Beziehung $(E,\vec{p}) = \hbar(\omega,\vec{k})$ verallgemeinern können, aus $E^2/c^2 - \vec{p}^2 = m^2c^2$ also $\omega^2/c^2-\vec{k}^2 = \kappa^2$ für eine Materiewelle schliessen können. Aber Einstein war mit der Gravitationstheorie genügend beschäftigt."[17] This argumentation is, however, unhistorical and theoretically untenable: even if Einstein, or somebody else, had constructed the formula $\omega^2/c^2 - \vec{k}^2=\kappa^2$, this would have had nothing to do, in itself, with matter waves. That Einstein did not conceive matter waves because he was too busy with gravitation theory is plain nonsense; this preoccupation didn't prevent him from delving intensively into quantum statistics in 1923-25.

Another story, which is subject to the same kind of objection, is Max Born's claim that he could have had "the whole wave mechanics from quantum mechanics at once, a few months before Schrödinger."[18] At another occasion Born has told his story as follows:

> "We [i.e. Born and Wiener]... published a paper which in some ways is a precursor of Schrödinger's operator calculus in quantum mechanics, but we just missed the most important point in a way which makes me ashamed even to this day. For in our paper we used the differential operator $D = d/dt$ and identified it with $(2\pi i/h)W$, where W denotes the energy, but we failed to see that in the same way d/dq represents $(2\pi i/h)p$, where p is the momentum belonging to the coordinate q. --- Thus we were quite close to have wave mechanics but we didn't reach it --- it was the most outstanding example of my being quite close to an important discovery and letting it slip by."[19]

What Born and Wiener would have obtained, would perhaps have been an operator formalism equivalent to wave mechanics, but it would by no means have been a wave mechanics in Schrödinger's sense.[20]

§ 2. FROM DE BROGLIE TO SCHRÖDINGER UNTIL CIRCA NEW-YEAR 1926.

As is well known, de Broglie's ideas were not received favourably by the physical community at their emergence in 1923-24. Outside Paris, they were largely ignored. One of those who fully appreciated de Broglie's theory, was Paul Langevin who spoke about it with sympathy at the Solvay Congress in 1924.[21] Langevin, who was one of the examiners of de Broglie's doctoral thesis, was a staunch relativist and was particularly impressed by the theory's founding on relativistic principles of invariance. It was also Langevin who sent a copy of de Broglie's thesis to Einstein in December 1924. Einstein hesitatingly recognised the importance of de Broglie's work,[22] and then backed it up with his full authority. In particular Einstein referred very positively to de Broglie's approach in his important work on gas degeneracy, issued on 9 February 1925.[23] It was this paper of Einstein's, and also a summary report appearing earlier in *Philosophical Magazine*,[24] which really made de Broglie's ideas known to people outside Paris. And it was also Einstein's gas theory paper which induced Schrödinger, at that time a professor at the University of Zürich, to study de Broglie's theory.[25]

According to the memory of Edmond Bauer,[26] Schrödinger received, at about the same time as Einstein, a copy of de Broglie's thesis which he did not, however, find reasonable ("that's rubbish!" Schrödinger is to have said). Only after Langevin had again advocated de Broglie's theory, Schrödinger took it up and realized its value to atomic theory. However, this story is not reliable since there is documented evidence that Schrödinger did not occupy himself with an extensive study of de Broglie's theory until November 1925 (see below). Anyhow, it was about February 1925 that

Schrödinger, inspired by Einstein, became acquainted with de Broglie's thinking, although at that time not with his major work, the thesis. Schrödinger's primary concern during 1925 was not in atomic theory but in the field of gas statistics, and consequently it was the gas statistical aspects of de Broglie's work which appealed to him. Schrödinger followed up Einstein's and Bose's pioneering theories in a number of investigations. During this period he appears to have been close to Einstein's research programme, in which proper atomic theory had only a remote placing. Schrödinger's works on quantum statistics have been thoroughly discussed by historians of science,[27] and shall not be mentioned here; also, they are largely unrelated to the genesis of Schrödinger's wave equation, which is our main concern. Suffice to say that Schrödinger, through the gas statistical approach, and particularly so in his *Zur Einsteinschen Gastheorie*, proceeded substantially towards the ideas of wave mechanics. In this paper Schrödinger made explicit use of de Broglie's formulae (1.2) and (1.4) for his phase waves. Concerning the energy spectrum of an ideal gas, Schrödinger wrote:

> "Wir berechnen es in engem Anschluss an L. de Broglie aus der Vorstellung, dass ein mit der Geschwindigkeit $v = \beta c$ bewegtes Molekül von der Ruhmasse m nichts weiter ist als ein 'Signal', mann könnte sagen 'der Schaukamm', eines Wellensystems, dessen Frequenz ν in der Nachbarschaft von
>
> $\nu = \frac{mc^2}{h\sqrt{1-\beta^2}}$ liegt und für dessen Phasengeschwindigkeit u ein Dispersionsgesetz gilt, das durch vorstehende Gleichung, in Verbindung mit $u = c/\beta = c^2/v$ gegeben wird."[28]

But wave mechanics, such as presented by Schrödinger in the spring of 1926, is essentially a theory of atoms, starting with the crucial case of the hydrogen atom. Wave mechanics was first really conceived when Schrödinger directed his interest towards an application of de Broglie's ideas to the hydrogen atom.

When de Broglie's thesis appeared in print, Peter Debye, then a professor at the Technical University in Zürich, received a copy and it was decided to take de Broglie's theory up at one of the joint physics colloquia which were regularly taken place together with physicists from the nearby University of Zürich. It may well have been, such as claimed by Debye many years after,[29] this colloqium which really opened Schrödinger's eyes to the use of matter waves in understanding atomic structure. "We were talking about de Broglie's theory", Debye recalled, "and agreed that we didn't understand it, and that we should really think about his formulations and what they mean. So I asked Schrödinger to give us a colloquium. And the preparation of that really got him started."[30] We may then assume that Schrödinger was asked to report on de Broglie's theory with which he was already fairly well acquainted and with which he had a professional and intellectual sympathy. Schrödinger prepared for the colloqium by a close study of de Broglie's thesis, published in *Annales de Physique*.[31] The same thing is reported by Erwin Fues (see § 5) and also by Felix Bloch, who attended the colloquia as a young student. Bloch remembers Debye saying something like: "Schrödinger, you are not working right now on very important problems anyway. Why don't you tell us some time about that thesis of de Broglie, which seems to have attracted some attention." When Schrödinger, in one of the next colloquia, had finished his account of de Broglie's theory, "Debye casually remarked that he thought this way of talking was rather childish. As a student of Sommerfeld he had learned that, to deal properly with waves, one had to have a wave equation. --- Just a few weeks later he [Schrödinger] gave another talk in the colloquium which he started by saying: "My colleague Debye suggested that one should have a wave equation; well, I have found one!""[32]

Whatever the historical accuracy of these reminiscences, it is a fact that Schrödinger, in the autumn of 1925, had completed a thorough study of de Broglie's thesis. On 3 November Schrödinger wrote to Einstein: "Mit grösstem Interesse habe ich vor einigen Tagen die geistvollen Theses von Louis de Broglie gelesen, deren ich endlich habhaft wurde."[33]

During this reading, Schrödinger noticed a striking similarity between de Broglie's resonance interpretation of the quantization conditions and an earlier theory of his own, in which he had attempted to reproduce the quantum conditions of the hydrogen atom from Weyl's extension of general relativity.[34] This work has been the subject of a detailed historical treatment by Raman and Forman,[35] who have suggested that the resemblance to de Broglie's ideas did not only affect Schrödinger's receptivity to de Broglie's thinking, but in fact determined the starting point for Schrödinger's attempt to develop de Broglie's theory into a wave mechanics of atoms. That Raman and Forman's suggestion is correct is, apart from their own careful argumentation, substantiated by the above mentioned letter which continues:

> "damit ist mir auch der § 8 Ihrer zweiten Entartungsarbeit erst voll deutlich geworden. Die de Brogliesche Interpretation der Quantelnregeln scheint mir Beziehungen zu haben zu meiner Note Zs.f.Phys. 12, 13, 1922, wo eine merkwürdige Eigenschaft des Weyl'schen "Massfaktors" $e^{-\int \varphi_i dx_i}$ entlang jedes quasi-periode gezeigt wird. Der rechnerische Sachverhalt ist, so viel ich sehe, derselbe, nur von mir viel umständlicher, weniger elegant, und nicht eigentlich allgemein gezeigt. Natürlich ist überhaupt de Broglies Ueberlegung in Rahmen seiner gros-

> sen Theorie von ungleich höherem Wert als meine Einzelfeststellung, mit der ich zunächst nichts anzufangen wusste."[36]

What seems important by Schrödinger's autumn study of de Broglie's thesis, is that his interest in de Broglie's work became no longer limited to gas theory, i.e. the Einstein programme, but from now on also covered atomic problems. On the other hand, Schrödinger did not at once concentrate on his new ideas on a wave mechanics of atoms at the expense of gas theory, which subject remained essential to Schrödinger. As is witnessed by the first part of the letter to Einstein, and as has been pointed out by Hanle,[37] Schrödinger continued to study de Broglie's theory in large measure to analyze Einstein's theory of quantum gas statistics.

A further impression of the state of affairs at about the assumed time of the Zürich colloqium may be gained from a letter to Landé of November 16:

> "Ich habe mir dieser Tage stark mit Louis de Broglies geistvollen Theses beschäftigt. Ist ausserordentlich anregend, hat aber doch noch sehr grosse Härten. Ich habe vergebens versucht, mir von der Phasenwelle des Elektrons auf der Keplerbahn ein Bild zu machen. Als "Strahlen" kommen doch wohl benachbarte Keplerellipsen von gleicher Energie in Betracht. Das gibt aber greuliche "Brennlinien" oder dergl. für die Wellenfläche."[38]

This letter seems to indicate that at this time, Schrödinger had taken the first hesitating steps towards an application of de Broglie's ideas to atomic structure and that these steps were a little prior to Schrödinger's application of the same ideas to gas theory. As pointed out by Wessels,[39] there is no mentioning of gas theory in the letter, such as one would expect to be the case if Schrödinger at that time worked on the ideas which were later published as *Zur Einsteinschen Gastheorie*. Wessels argues, furthermore, that Schrödinger's remarks about 'greuliche "Brennlinien"' ('horrible caustics') indicate that Schrödinger was then still following de Broglie's conception of matter waves as travelling waves. In contrast, the picture Schrödinger outlined in his wave mechanics, was one of standing waves and this idea, crucial to the whole wave mechanics, had not as yet entered Schrödinger's mind.

Probably Schrödinger was on the track of the basic features of wave mechanics in late November and has worked parallelly on this new trend and on his theory of gas statistics. The latter work may have occupied most of Schrödinger's resources, so it was only after mid December he was able to concentrate on the new approach to atomic theory; and to do so with an increasing intensity.

Schrödinger's attempt to apply a standing wave modification of de Broglie's theory to the hydrogen atom resulted in a wave equation, which Schrödinger presumably had found at about mid December. This differential equation was, as will be substantiated in the latter part of this article, the relativistic wave equation. Schrödinger's efforts culminated during a christmas vacation in Arosa in Italy. On 27 December he wrote to Wilhelm Wien and told about his progress as well as about his difficulties:

> "Im Augenblick plagt mich eine neue Atomtheorie. Wenn ich nur mehr Mathematik könnte! Ich bin bei dieser Sache sehr optimistisch und hoffe, wenn ich es nur rechnerisch bewältigen kann, so wird es sehr schön. Ich glaube, ich kann ein schwingendes System angeben - u. zw. auf verhältnismässig natürlichen Wege, nicht durch *ad hoc* Annahmen - das die Wasserstofftermfrequenzen zu Eigenfrequenzen hat. Aber nicht eigentlich diese selbst, also nicht
> $-{}^{R}/n^{2}$, sondern $\frac{mc^2}{h} - \frac{R}{n^2}$ (m = Elektronenmasse).
> Diese Frequenzen sind sehr hoch gegen die optischen und auch noch gegen die Röntgenfrequenzen haben aber nuhr sehr kleine relative Differenzen voneinander. Daher ist, wenn etwa

$$\nu_n = \frac{mc^2}{h} - \frac{R}{n^2}, \qquad \nu_m = \frac{mc^2}{h} - \frac{R}{m^2}$$

als dann

$$\nu_n - \nu_m = R\left(\frac{1}{m^2} - \frac{1}{n^2}\right)$$

eine richtige Schwebungsfrequenz. Damit ist ein wirkliches Verständnis der Bohr'schen Frequenzberechnung angebahnt - es ist wirklich ein schwingungs - (bezw. ein Schwebungs)vorgang da, welcher mit derjenigen Frequenz erfolgt, die wir im Spektroskop beobachten.

Ich hoffe, ich kann bald ein wenig ausführlicher und verständlicher über die Sache berichten. Vorläufig muss ich noch Mathematik lernen, um das Schwingungsproblem ganz zu übersehen - eine lineare Differenzialgleichung, der Bessel'schen ähnlich, aber weniger bekannt und mit merkwürdigen Randbedingungen, welche sie "in sich trägt", nicht von aussen vorgeschrieben bekommt."[40]

From this interesting letter it seems justified to infer that at the end of December Schrödinger was still occupied with a relativistic formulation (cf. the mc^2 terms); he had found the eigenvalue equation for the hydrogen atom, but had not as yet been able to solve it because of mathematical difficulties. Schrödinger's hints at a wave explanation of Bohr's frequency condition in terms of beats (*Schwebungen*) was taken up in his first communication on wave mechanics, submitted for publication exactly one month later. In there, Schrödinger virtually echoed the remarks in the letter to Wien.[41] At an earlier date, also de Broglie had considered Bohr's frequency condition as a kind of a beat relation, resulting from interfering phase waves belonging to the two energy levels in question.[42] Although this consideration is not included in the *Thèse*, Schrödinger may have been acquainted with de Broglie's idea.

Schrödinger remained in Arosa until 9 January 1926. A few days after his return to Zürich, he succeeded to solve his wave differential equation for the hydrogen atom, although with a rather disappointing result. Before proceeding with Schrödinger's early treatment of the hydrogen atom we shall, however, make a somewhat lengthy digression on the role of the hydrogen spectrum in quantum theory.

§ 3. THE HYDROGEN SPECTRUM IN QUANTUM THEORY.

In the development of modern atomic theory the hydrogen spectrum has played a unique role. Ever since Balmer and other scientists in the late nineteenth century expressed the regularities of the hydrogen spectrum by simple formulae, the hydrogen spectrum had a profound impact on the advance of atomic theory. The history of the role of the hydrogen spectrum remains to be written.[43] What follows, is not an attempt to do so, but merely an outline of some spectacular events connecting the hydrogen spectrum to quantum theory. It is intended to furnish a background for the further account of relativistic quantum mechanics in which the hydrogen spectrum played a central role. In this section I shall deal briefly with the hydrogen spectrum before quantum mechanics, while in the next section I shall consider the earliest quantum mechanical attempts to quantize the hydrogen atom.

As is well known, Balmer's formula from 1885 was succesfully explained by Niels Bohr in his atomic theory from 1913. Bohr stated Balmer's formula by means of the expression

$$E_n = - \frac{2\pi^2 e^4 m Z^2}{h^2} \cdot \frac{1}{n^2} \qquad (3.1)$$

with Z=1 for hydrogen, and n=1,2,3... being the principal quantum number. The relation to the empirical Balmer formula is obtained by putting R (Rydberg's constant) equal to $2\pi^2 e^4 m h^{-2}$ and by Bohr's second postulate $(E_n - E_m) = h\nu$, where m = 2 for the Balmer series. Bohr's theory was not really a theory of the hydrogen atom. In fact, the major part of the theory was worked out in 1912, at a time when Bohr did not at all consider, and had not yet taken note of, Balmer's formula.[44] This is noteworthy, because the acceptance of Bohr's ideas relied to a high degree on his derivation of Balmer's formula and on further details concerning the hydrogen spectrum. This was, so to speak, the point which made otherwise sceptical physicists swallow Bohr's strange theory. From that time on, and also at some previous occasions (for example, the pre-Bohr attempts of Haas, Schidlof and Herzfeld to introduce the quantum of action in atomic structure) the hydrogen spectrum became the issue upon which new atomic theories were judged. As the simplest physical system in nature, the hydrogen atom became a test case for new quantum theories' reliability as regards physical reality.

Already at the arrival of Bohr's theory, it was known that the simple Balmer expression, and then eq.(3.1), did not entirely reproduce the visible part of hydrogen's spectrum. In 1891 Michelson had detected a small deviance from Balmer's formula, indicating a doublet structure of the individual lines with a separation in wave number of circa 0.3 cm^{-1}, and in 1914 Curtis reported the same disagreement more systematically. The lack of precise agreement between Bohr's theory and experimental spectroscopy called for a refinement of Bohr's atomic model, originally formulated non-relativistically. In 1915 Bohr therefore considered the relativistic change of mass with velocity, and he obtained an extra frequency which narrowed the gap between theory and experiment, but did not remove it.[45]

A full inclusion of special relativity in Bohr's atom was attained with Sommerfeld's theory from 1915-16. According to Sommerfeld the relativistic motion of an electron in a Coulomb field was fully described (in the case of no external magnetic field) by two quantum numbers, n and k. The quantization procedure applied by Sommerfeld yielded the following, rigorous formula for the energy levels:

$$E_{n,k} = m_0c^2\left\{1 + \frac{\alpha^2 Z^2}{[(n-k) - \sqrt{k^2-\alpha^2 Z^2}]^2}\right\}^{-\frac{1}{2}} - m_0c^2 \qquad (3.2)$$

Here α is Sommerfeld's fine-structure constant $2\pi e^2h^{-1}c^{-1}$, n is Bohr's principal quantum number and k is the azimuthal quantum number, $k = 1,2,\ldots,n$. Instead of using n and k, the formula was often written in terms of n_r and k, where n_r is the so-called radial quantum number, $n_r = (n - k)$. An expansion in powers of $(\alpha Z)^2$ gives the following, more workable expression:

$$E_{n,k} = -\frac{RhZ^2}{n^2}\left[1 + \frac{\alpha^2Z^2}{n^2}\left(\frac{n}{k} - \frac{3}{4}\right)\right] \qquad (3.3)$$

In the following, this formula will be called the 'approximate Sommerfeld formula', while (3.2) is the 'exact Sommerfeld formula'. Sommerfeld's theory was brilliantly confirmed right after its appearance, especially by the experiments made in Tübingen by Paschen and his co-workers. In 1916, Paschen's measurements of the doublet separation in the H_α line indicated a value of 0.31 cm^{-1}. In comparison, the theoretical value obtained from (3.3) is

$$\Delta\nu = \frac{1}{h}\Delta E = \frac{R\alpha^2 Z^4}{16} = 0.3650 \text{ cm}^{-1}$$

From continued measurements, the Tübingen spectroscopists reported in 1924 their best result to be $\Delta\nu = (0.3645 \pm 0.0045)$ cm^{-1}, i.e. a perfect agreement.[46] The bulk of Paschen's measurements focussed on the lines of ionized helium, particularly on the wavelength 4686 Å, due to the transition $n=4 \rightarrow n=3$. It was this line, rather than the H_α line, which became a kind of test case for the theory (the advantage of using He^+ instead of hydrogen as a test is, of course, due to the factor Z^2 which makes the He^+ separation sixteen times that of hydrogen). Sommerfeld's theory showed equally valuable to the study of X-ray spectra, and also in this area it appeared to predict the experimental data with excellent accuracy.[47] All things considered, the evidence in support of Sommerfeld's theory were so impressive that very few physicists doubted the correctness of the explanation of the hydrogen spectrum in terms of relativity. What appeared to be a perfect agreement between theory and experiment convinced theoretical physicists that the hydrogen spectrum was no longer a problem and was therefore hardly worth to investigate any further. This feeling was only strengthened by the demonstration that the theory was able to account also for the behaviour of an electron placed in a crossed electric and magnetic field.[48]

In this way the success of Sommerfeld's explanation turned out to have, from a retrospective point of view, a repressive impact upon the development of atomic physics, rather than a progressive one. As was only clarified some 12 years later, the agreement is largely coincidental, since Sommerfeld's relativistic explanation by chance includes the effects of spin, unknown in 1916. This accurate agreement was, in Van Vleck's words, "perhaps the most remarkable numerical coincidence in the history of physics";[49] and Kronig has called it "a fortunate coincidence".[50] A coincidence it was, but one may wonder if it was really a fortunate one or if it was not rather a hindrance, as the troubles became disguised in the remarkable agreement. If the relativistic treatment of the old quantum theory had not given this extraordinary result, the hydrogen case would still have been regarded as an anomaly. Being the most simple atom, an explanation of its spectrum would have been a challenging problem to the theorists and would probably have resulted in new insights. Of course it is impossible to say what would have happened if the course of history had been different, but in this case one would assume that the collapse of the old quantum theory and the emergence of the new quantum mechanics would have accelerated. The role of a 'hydrogen puzzle' would probably have been even greater than other experimental anomalies, such as the anomalous Zeeman effect and the helium spectrum.

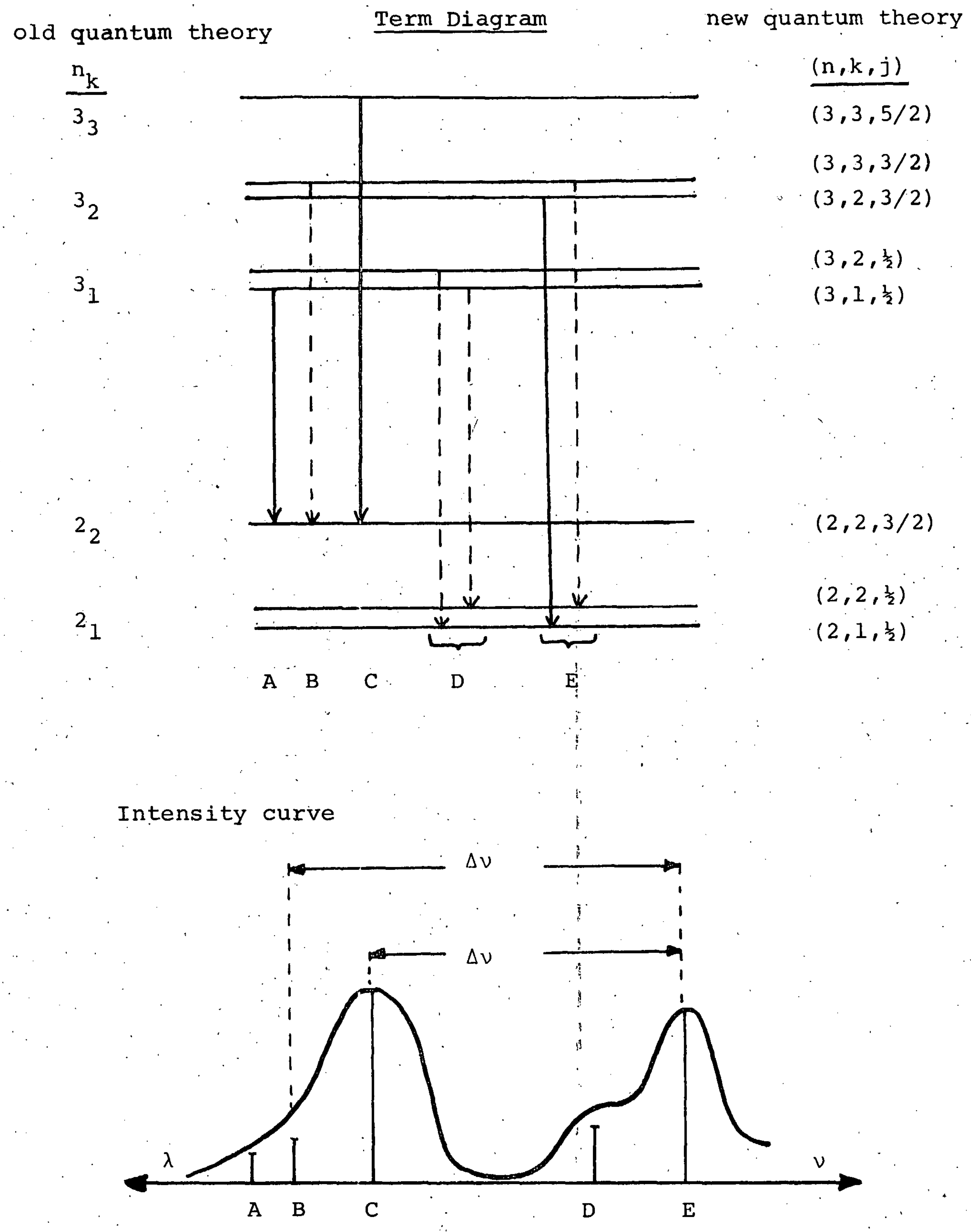
The situation being as it was, the interest was turned away from the simple spectra of hydrogen and He^+, and it was in connection with more complicated spectroscopic phenomena - Zeeman effect, doublets and multiplets in the optical region and in the X-ray region - that the dissolution of the old quantum theory took its beginning. From 1925 it became, furthermore, increasingly realized that not even for the hydrogen spectrum could Sommerfeld's theory be regarded as the final word. This insight was gradually forced upon by new measurements of the fine-structure of the Balmer lines. Most of these measurements took advantage of the newly developed plates of Lummer and Gehrcke which allowed a better resolution than in Paschen's classical observations, based on optical gratings. In 1924-26 several German spectroscopists challenged Paschen's measurements and reported values for the doublet separation in H_α which were considerably lower than predicted by Sommerfeld's formula. Janicki, Lau, Gehrcke a.o. concluded that $\Delta\nu$ was close to 0.306 cm^{-1} and that Sommerfeld's theory was therefore unable to account for the finer details of the hydrogen spectrum.[51] Other spectroscopists criticized these conclusions and claimed that the measurements either supported Sommerfeld's theory or that they were inconclusive.[52] On the whole, there was wide disagreement among the best German spectroscopists about how to interpret the experiments.

Spectroscopic precision measurements on the fine-structure in hydrogen were met with serious experimental difficulties, which made the data rather unrealiable as a test of Sommerfeld's theory. The difficulty is in particular due to the widening of the spectral lines caused by the Doppler effect; at room temperature the Doppler width of the H_α components is about 0.2 cm^{-1}, which will effectively prevent a satisfactory resolution of the spectral lines. Apart from the experimental difficulties, the disagreements about the hydrogen fine-structure were also rooted in confusion about the proper interpretation of the experimental results. The 'idealized' H_α doublet, $\Delta\nu$, is the difference between the 2_2 and 2_1 levels (using a n_k notation) which is not, however, directly observable. The observed values reported by the spectroscopists were the difference between the two observable peaks of the doublet; and this value is only identical to the theoretical $\Delta\nu$ if the fine-structure of the n=3 levels is disregarded. From the three transitions, allowed to occur according to the old quantum theory, $\Delta\nu$ cannot be exactly determined (see the figure).

In this development, the careful observations of G.Hansen on the Balmer lines were of particular importance.[53] Hansen reported not only a $\Delta\nu$ of 0.318 cm^{-1}, i.e. much below the Sommerfeld-Paschen result, but more important, he reported observation of a new line which could only be ascribed to the transition $3_1 \rightarrow 2_1$ (D in the figure). This component, for which there was soon found additional evidence,[54] is forbidden according to the Bohr-Sommerfeld theory: In there, transitions are governed by the selection rule

$$\Delta k = \pm 1$$

such as Bohr had demonstrated in 1918 from the correspondence principle. The fine-structure of the H_α line 6563 Å consists, then, of only three lines according to the Bohr-Sommerfeld theory (indicated with full lines in the figure). Experimentally, they appear as a doublet because the n=3 levels are very close to each other; the two transitions from n=3 to $n_k=2_2$ (A and C) cannot be resolved, and appear as a singlet. So there was no room for further lines if keeping to the traditional quantum notation and selection rules. The interpretation of the new



THE H_α SPECTRUM

lines found in hydrogen, and also in He^+, as well as the experimental confusion as regards the value of the fine-structure separation, therefore presented a dilemma to Sommerfeld's relativistic treatment of the Bohr atom. The evidence from the hydrogen spectrum, however came at a relatively late date, about the autumn of 1925, at a time where many other evidences clearly called for a revision of the old quantum theory's spectroscopic results (see below).

The answer to the dilemma was at first purely formal, consisting in a relabelling of quantum states and a revision of selection rules. The merits of Sommerfeld's theory for hydrogenic atoms were, after all, too impressive to allow the theory to be invalidated by experimental evidences of a not too conclusive nature. There were, however, some attempts to formulate alternative quantum theories for the hydrogen atom. These attempts came at a time where the new quantum mechanics had already invalidated the foundation of Sommerfeld's theory, although without being able to furnish a satisfactory explanation of the spectral fine-structure. They were therefore outdated at their very emergence and they were not, at any rate, regarded to be serious alternatives. Nevertheless, these attempts from the fringe of mainstream physics should not be ignored in a historical context.

M.Bronstein, a physicist from Kiev, proposed to build up a theory of spectral fine-structure based on a dubious modification of relativistic mass variability.[55] He proposed to replace the usual relativistic expression for the mass of an electron in a Coulomb field

$$m = \frac{m_0}{\sqrt{1-\beta^2}} - \frac{e^2}{c^2 r}$$

with

$$m = \frac{m_0 - \frac{e^2}{c^2 r}}{\sqrt{1 - \beta^2}}$$

i.e. to include the potential energy of the electron in the rest mass. From this approach, and by following Sommerfeld's integration procedure from 1916, Bronstein derived a fine-structure formula which only differed from Sommerfeld's with the close to one factor $(1 - {}^{2m}o/m_o')$, where m_o' is the rest mass of the hydrogen nucleus. However, as quickly pointed out by Kudar,[56] Bronstein's speculative theory has nothing whatsoever to do with proper relativity theory, and the almost-agreement with Sommerfeld's result hence was without any scientific importance. Sommerfeld's theory of fine-structure was also challenged by Adolf Bucherer, then honorary professor in Bonn, who adopted Bronstein's view of including potential energy in the rest mass.[57] Bucherer's theory was no less artificial than Bronstein's, and neither it seems to have been taken seriously by other physicists. In contrast to Bronstein, Bucherer deduced a widely different fine-structure splitting than in Sommerfeld's theory, namely $\Delta\nu = 0.296\ \mathrm{cm}^{-1}$. From this value, compared with the recent measurements of Gehrcke, Lau a.o., Bucherer felt justified to conclude that his own theory was superior to Sommerfeld's, and that the standard interpretation of relativity theory hence was shown to be inadequate.

The attacks on Sommerfeld's explanation of fine-structure were, in large measure, connected with the attacks on Einsteinian relativity, which were fairly frequent in the twenties, particularly among the 'right wing' physicists in Germany. Much of the critique launched against Einsteinian relativity had political and racial overtones, especially the part associated with the viewpoints of Lenard and Stark.[58] Bucherer belonged to the group of elder professors, who were not able to accept relativity in Einstein's key.[59] In this context, it may also be relevant to point out that Eduoard Gehrcke, a noted specialist in optics and one of the physicists who reported fine-structure values incompatible with Sommerfeld's theory, shared the anti-relativist stand of Bucherer, Lenard a.o. Just as Bucherer, Gehrcke had for years criticized the theory of relativity, partly from philosophical grounds and partly from the standpoint of an experimental physicist's.[60]

It should not be forgotten, however, that in spite of the numerous attacks on Einsteinian relativity in the twenties, this trend did not penetrate into the mainstream of physics to any considerable extent. In Göttingen, Berlin, Hamburg, Zürich and Copenhagen, the anti-relativists were, in no small measure, considered to be a group of quasi-cranks.

But let us return to the so-called mainstream of development. As previously mentioned, it was particularly investigations of alkalidoublets and of X-ray doublets which in 1925 led to a general distrust in Sommerfeld's theory, not evidences from the simple spectra of hydrogen and He^+. The entangled story has been analysed in details by Forman and by Serwer, to whome is referred for further information.[61]

In early 1924 Millikan and Bowen had casted serious doubts on Sommerfeld's relativity explanation of the doublet structure of spectra.[62] By extending Sommerfeld's formula for X-ray doublets to optical spectra, the two American physicists pointed out a number of difficulties to the Bohr-Sommerfeld theory which indicated that the empirical material could not be accounted for by means of the theory's conception of relativity doublets.

Millikan and Bowen simply proposed:

> "to throw overboard altogether the relativity explanation of the "relativity-doublet" and to assume that the amazing success of this relativity formula in predicting the correct numerical values of s [i.e. the screening constant] .... is not at all due to differences in the shapes of elliptical and circular orbits, as postulated by the relativity theory of doublet separations, but that there is some other cause which by mere chance leads exactly to this relativity formula without actually necessitating relativity conceptions."[63]

They were not able to concretize their critique any further than presenting a dilemma, both of which two horns seemed well-founded: either relativity effects had to be abandoned altogether in electronic orbits, or Bohr's ideas of penetrating orbits and the standard assignment of quantum numbers had to be abandoned. In another paper,[64] written half a year later, Millikan and Bowen suggested an escape from the dilemma by proposing that there was a qualitative difference between the explanation for doublet-spectra of hydrogen and He^+ on the one side and for all the other spectra on the other side. This suggestion of a qualitative break implied what they called "a very difficult and strange assumption", viz.:

> "that the remarkable fitting of all our data into the relativity formula for all the atoms from lithium up to chlorine, and then throughout the whole X-ray field, is accidental, and that there must be some other cause of a non-relativistic sort which is responsible for the behaviour of the spectra of all these elements."[65]

Millikan and Bowen tried to justify their suggestion of a break between helium and lithium with various spectroscopic evidences but had, in the end of their paper, to appeal to the atomic theorists for assistance: "To find a new cause for the relativity-doublet-formula...... is a problem worthy of the efforts of the theoretical physicist."[66] The call had already been answered by Landé, who tried to avoid relativistic explanation of the X-ray doublets altogether and to ascribe them to a magnetic interaction instead of. However, Landé's attempt failed.[67]

As is quite clear from Millikan & Bowen's critical review, anticipating much of the development to come, the critique was not directed towards Sommerfeld's theory for the *hydrogen* atom. In 1924 there was still an almost unshakable faith in the correctness of the relativity formula so far as hydrogen and He^+ was concerned. This faith became almost a dogma which for a time prevented the physicists to take serious the evidences for disagreement between theory and experiment in the hydrogen spectrum. Such evidences of anomalies were neglected or explained away. There was, for example, the problem of Paschen-Back effect in the H_α lines: The Bohr-Sommerfeld theory had well accounted for the experimental fact that while the components of the hydrogen-spectrum (or He^+ spectrum) show a normal Zeeman effect, lithium and higher atoms show anomalous Zeeman effect. According to the theory, the so-called Paschen-Back effect (i.e. the change towards a normal Zeeman pattern under strong magnetic fields) was excluded in the case of hydrogen. However, in 1922 Oldenberg[68] had reported evidence for Paschen-Back effect also in H_α, an observation which was substantiated the following year by Hansen and Försterling.[69] In 1926 Sommerfeld and Unsöld correctly, although with the advantage of hindsight, called this evidence "einen der ernsteten Einwände gegen die bisherige Theorie des Wasserstoffatoms".[70] But before that time the anomaly was largely ignored or even forgotten. Goudsmit and Uhlenbeck, for instance, seemed not to have been aware of it in the autumn of 1925,[71] and Millikan and Bowen chose to consider the evidence for Paschen-Back effect as inconclusive. The mentioned anomaly, and the way in which it was treated by the physicists, is, on the whole, a fine example of Kuhn's idea of the role of anomalies under normal periods of science.[72]

To make a long story short, the difficulties which had accumulated as regards the interpretation of alkalidoublets and X-ray spectra eventually led also to a reconsideration of hydrogen's spectrum. In August 1925 Goudsmit and Uhlenbeck proposed to conceive the fine-structure of hydrogen as though it was a special case of an alkali doublet.[73] From this standpoint they suggested a new term structure with new selection rules. A similar suggestion was made by Slater a few months later[74] and had previously been proposed also by Landé (but not published).[75] But it was first in 1926, when Sommerfeld and Unsöld reexamined the whole matter,[76] that the new classification scheme was generally accepted (Goudsmit and Uhlenbeck's paper was written in Dutch in a not widely circulated journal). At this time, the spin hypothesis had been introduced and the new quantum mechanics applied to the hydrogen atom by Pauli and by Dirac.

Sommerfeld and Unsöld calculated the intensities of the five H_α lines which were allowed according to the new classification. This was done, in accordance with the suggestion of Uhlenbeck and Goudsmit, simply by applying the semi-empirical intensity rules of the alkali and X-ray spectra. The calculated intensities showed a better agreement with experiments than did the intensities calculated from the old quantum theory (based on Kramers' extension of Bohr's correspondence principle). Sommerfeld and Unsöld ended their paper: "Die relativistischen Formel bleibt für Wasserstoff-, Röntgen- und sichtbare Spektren erhalten, aber ihre modellmässige Grundlage scheint der empirisch erforderlichen Quantenbezifferung zu wiedersprechen."[77] In the very accurate analysis of the hydrogen spectrum, made by Kent et.al. in Boston in the beginning of 1927, a best value for the hydrogen doublet separation was found to be (0.318 ± 0.002) cm^{-1}, in good agreement with Hansen's result, and also in fair agreement with the value predicted by the new spin quantum theory. As to the number of lines compositing the intensity curve, they concluded:

> "... we feel justified in stating that with H_α and H_β the resultant curves are not inconsistent with the presence of the five components given by the new quantum mechanics with the spinning electron. Of the presence of c' [D in our figure] we are certain; we are reasonably sure of b'' [B]; and, lastly, the resultant curves fit the case better *with* c'' [A] than without it."[78]

In the new picture of the hydrogen spectrum, the energy levels were assigned new labels, now by three quantum numbers. Apart from n and k, also used in Sommerfeld's original theory, the inner quantum number j, was taken over from X-ray classification. According to the new ideas, the 3_2 level now consisted of two (coinciding) levels, $(n,k,j) = (3,3,3/2)$ and $(3,2,3/2)$, and similarly for the other levels; cf. the figure. Together with the new classification scheme, new selection rules were provided. Transitions for which

$$\Delta k = \pm 1 \quad \text{and} \quad \Delta j = \pm 1, 0$$

were now allowed. This yields two extra components, of which one (due to $(3,2,\frac{1}{2}) \rightarrow (2,1\frac{1}{2})$) accounted for Hansen's observation. In the new picture, then, the two peaks of the intensity curve were composited by two and three lines, respectively. The difference between the peaks corresponds approximately to the difference between $3_2 \rightarrow 2_1$ and $3_3 \rightarrow 2_2$, which is not identical to $\Delta\nu = 2_2 - 2_1$. $\Delta\nu$ may be got as the difference between $3_2 \rightarrow 2_1$ and $3_2 \rightarrow 2_2$, where the latter is a new line. This line, however, is not identifiable in the larger wavelength component. In itself, Sommerfeld's formula was left untouched, that is, the number of different energy levels as well as their term values were not changed. If Sommerfeld's original formula should conform to the new scheme, its azimuthal quantum number k should be substituted with $j+\frac{1}{2}$. Since j is a half-integer, this leaves the validity of Sommerfeld's formula unchanged.

Most of the new development is hydrogen's "term-zoology" was of a purely formal character and did not consider any physical explanation of the mechanisms of the spectra. In early 1925 Kronig had informally introduced the spin hypothesis by assuming the electron to have an intrinsic angular momentum due to its spinning about its own axis. His idea was put forward only to be ridiculed by Pauli and rejected by Heisenberg and Kramers, and thus it never appeared in print. Kronig's idea was independently worked out by Uhlenbeck and Goudsmit in two short papers from 1925 and 1926 and gradually won acceptance despite of its weaknesses and lack of theoretical justification. How this development took place has been analysed in details by historians and by the involved physicists.[79]

At the start of 1926 the spin hypothesis had been generally accepted, not least because of Bohr's endorsement. Some physicists, in particular Pauli, still would not know about spinning electrons and they had good reasons for their scepticism. The assigned magnetic moment of one Bohr magneton seemed incompatible with the then predominant view of the nucleus as consisting of protons and electrons. And if the spin model was to be taken at face value, the peripheral velocity of the spinning charge ball greatly exceeded, it was calculated, the velocity of light! But the gravest difficulty was the so-called riddle of the 2-factor: On Landé's core-model, it had been necessary in order to account for the socalled *g-formula*, to assume a gyromagnetic ratio (magnetic moment to angular moment) of twice the classical value of the core, that is, $^{e}/mc$ instead of $^{e}/2mc$. This assumption was taken over in the spin theory to explain the Zeeman effect quantitatively, but was now attributed to be a property of the rotating electron. There was, however, no proper theoretical justification for this assumption.[80] Just after Goudsmit and Uhlenbeck's first publication of spin, Heisenberg and Pauli calculated the separation for spin-doublets according to the spin hypothesis in the old quantum theory, and they found it to be twice as large as the experimentally observed values (see § 4). This annoying factor of two was only rectificated in March 1926 when Thomas calculated the precession of the spinning electron under consideration of relativity and showed that the spin-doublets then came out right.

§ 4. EARLY QUANTUM MECHANICS, RELATIVITY, AND THE HYDROGEN SPECTRUM.

When the new quantum mechanics appeared in the early autumn of 1925, its formalistic character and its strange mathematical language made it not immediatedly acceptable to most physicists. The Göttingen physicists' matrix mechanics was from many quarters accused of *Unanschaulichkeit*. Despite of the variety of physical problems to which the matrix mechanical methods were applied by Heisenberg, Jordan and Born (particularly: dispersion, harmonic and anharmonic oscillator, intensity rules for spectra), matrix mechanics in 1925 did not appear completely convincing from a empirical-physical point of view. What lacked, many people felt, was a demonstration that the matrix mechanical formalism was also able to deal with physical systems such as actually occuring in nature. If the new quantum mechanics should become accepted as superior to the old quantum theory, and also become accepted as a physically sound theory, it had to face the test case of the hydrogen atom. Early quantum mechanics' dilemma between formalism and physical applicability was clearly realized by the discoverers themselves, who at an early stage directed their interest towards the hydrogen spectrum: the new mechanics ought to be able to derive the simple Bohr formula for the Balmer lines, or, even better, to reproduce the complete spectral formula of Sommerfeld. However, since the latter was a result of - or, was thought to be a result of - relativity, and since matrix mechanics was a non-relativistic theory, the immediate goal was to deal with the Balmer terms.

It appears, furthermore, that only mathematical difficulties prevented the hydrogen atom to play a role as a test case in Heisenberg's creation of quantum mechanics, similar to the role played in the creation of wave mechanics. In the spring of 1925, Heisenberg started out by trying to apply his ideas about virtual oscillators to the hydrogen atom. It was only when this problem turned out to be too difficult that Heisenberg was forced to direct his attention to the anharmonic oscillator, physically being a more unrealistic, and then less attractive case than the hydrogen atom.[81] So even if the hydrogen atom does not appear in the pioneering articles from 1925, surely it played an important role also in the fabrication of the Göttingen mechanics.

In a paper submitted in January 1926, Pauli first succeeded to apply matrix mechanics to the hydrogen atom.[82] The publication of Pauli's paper appeared as a release to the scientists who were still not convinced about the physical soundness of matrix mechanics. Van Vleck's reminiscens may have been characteristic for a large part of the physical community of the time: "I eagerly waited to see if some one would show that the hydrogen atom would come out with the same energy levels as in Bohr's original theory, for otherwise the new theory would be a delusion. Finally Pauli's paper appeared which dispelled my worries."[83] Pauli's important paper was received by the *Zeitschrift* on 17 January 1926, but we know that its main results were obtained much earlier. On 3 November Heisenberg thus wrote to Pauli and told him "wie sehr ich mich über die neue Theorie des Wasserstoffs freut".[84] Heisenberg had himself attempted to apply his new concepts on the hydrogen atom, but had not succeeded. As he recalled: "Ich war damals [in the end of October 1925] etwas unglücklich darüber, dass es mir nicht gelingen wollte, auch nur das einfache Wasserstoffspektrum aus der Theorie abzuleiten.... Schon Oktober aber überraschte mich Pauli mit der vollständigen Quantenmechanik des Wasserstoffatoms."[85] (See also Heisenberg's letter to Dirac, excerpted below). So it seems certain that Pauli had obtained the Balmer formula from matrix mechanics already about late October 1925. In regard of the importance of this result, one of the uttermost importance for the acceptance of the new physics, why did Pauli delay its publication for almost three months?

There are good reasons to believe that the considerable delay was caused in an unsuccessful attempt of Pauli's to proceed beyond the derivation of the simple Balmer formula and to cope also with the fine-structure, i.e. to derive Sommerfeld's formula by a relativistic refinement of the theory. It was only after Pauli reluctantly had given up this attempt that he submitted his paper with the absence of relativity corrections. As we shall see below, the attempts to extend the non-relativistic matrix mechanics to cover also relativistic effects were not confined to Pauli; in Göttingen also Heisenberg and Jordan struggled with the problem. For Pauli's whole scientific outlook it was indeed natural to attack the hydrogen atom with the inclusion of relativity. Pauli was a noted expert on relativity theory and had already gained a reputation as a firm 'relativist' in questions concerning the interpretation of spectral doublets.[86] The assumption is substantiated by an examination of his paper.

We shall leave the technical details apart, which have been discussed by Van Vleck and van der Waerden.[87] Pauli's main result was the derivation of the Balmer formula, i.e. a quantum mechanical derivation of Bohr's result (3.1); he also used the oppotunity to give an explanation of the Stark effect, in good agreement with the experiments. Pauli had to admit, however, that his approach failed to account for the fine-structure of hydrogen and that it was also not able to reproduce the anomalous Zeeman effect. Even if a derivation of the fine-structure terms was outside the power of Pauli's theory, he was able to deduce the correct number of energy-levels, in accordance with Sommerfeld's theory. Pauli apparently had attempted to derive the fine-structure formula from a relativistic extension of his theory; the calculation of the relativistic energy correction, however, proved to be very difficult. Pauli writes:

> "Ob diese Annahme [Uhlenbeck and Goudsmit's spin hypothesis] ausreicht um im Verein mit der neuen Quantenmechanik alle Erfahrungsresultate zu erklären, dürfte sich erst entscheiden lassen, wenn auch die Berechnung der relativistischen Feinstruktur auf grund der neuen Mechanik durchgeführt ist. Diese blieb vorläufig noch ausser Betracht, da die hierzu erforderliche Berechnung des zeitlichen Mittelwertes $\overline{\frac{1}{r^2}}$ uns noch nicht gelungen ist."[88]

This remark shows that Pauli had in vain sought to obtain the approximative Sommerfeld formula: A relativistic treatment of the hydrogen atom shows[89] that the energy may approximately be written as

$$E = E_0 + E_1$$

E_0 is the classical energy and E_1 is a small correction, considered to be a perturbation, of the form

$$E_1 = -\frac{1}{2m_0c^2}\left\{E_0^2 + 2Ze^2E_0\left(\frac{1}{r}\right) + Z^2e^4\left(\frac{1}{r^2}\right)\right\} \qquad (4.1)$$

Quantumtheoretically, in the new quantum mechanics as well as in Sommerfeld's theory, the energy correction comes out as the mean value of E_1, taken over the undisturbed path. It was the problem of finding the latter mean value (or, quantum mechanically, the expectation value) that troubled Pauli.

In the winter of 1925-26 Pauli was still hostile to the idea of spin, and he wanted to treat the hydrogen atom without retreat to the spin hypothesis. He was aware, however, that the spin hypothesis might be the clue which could furnish an explanation of the anomalous Zeeman effect and of Sommerfeld's formula, recognised to be two sides of the same matter.

It was not only in Germany that quantum physicists were engaged in the attempt to deal with the hydrogen atom. In the beginning of 1926 Dirac in Cambridge submitted a paper in which he attacked the matter by means of his algebraic version of quantum mechanics.[90] Just as Pauli, Dirac succeeded, although by an entirely different method, to deduce the Balmer frequencies of the hydrogen atom. In contrast to Pauli, Dirac did not consider the case of the hydrogen atom in a magnetic field, and neither did he attempt to cope with the fine-structure. When Dirac worked out his theory of the hydrogen atom, he was aware of Pauli's work on the same subject. "I was really competing with him at this time," Dirac has recalled.[91] Already in November 1925 Dirac knew about Pauli's work, informed by Heisenberg: "Pauli has succeeded in getting the theory of the hydrogen atom and the Balmer formula on quantum mechanics. I would willingly send you proofs of this paper and would be glad to hear of your further progress," Heisenberg wrote.[92] Apparently, Heisenberg sent a proof of Pauli's paper, for Dirac mentions in a footnote that he has read a proof of it. If the publications of Dirac and Pauli are seen as the results of a competition, Pauli was no doubt the winner: Pauli's theory was not only a little prior to Dirac's , but it was also superior in respect of physical content. Dirac's theory of the hydrogen atom demonstrated, however, that his quantumalgebraic method was not devoid of physics; though appearing as a very formal and abstract scheme, it could be successfully applied to the hydrogen atom. This, no doubt, was the prime reason for Dirac's publication.

Even if the Pauli-Dirac derivation of the Balmer terms was an acknowledged success for the new quantum theory, it was not complete: it still lacked to reproduce the fine-structure, i.e. either the approximate Sommerfeld formula or, even better, the exact Sommerfeld formula. This task, only fulfilled with Dirac's electron theory from 1928, was the one Pauli had struggled with. It constituted an important theme in the entire development of quantum mechanics from 1925 to 1928.

Pauli's and Dirac's works on the hydrogen atom were further developed by Gregor Wentzel[93] by a method which was essentially a matrix mechanical version of Sommerfeld's 1916 theory. Wentzel first derived Balmer's formula in the form

$$E = \frac{2\pi^2 me^4}{(I_r + I_\varphi)^2}$$

Here, I_r and I_φ are action variables in Dirac's sense, corresponding to the old quantum theory's action integrals $\int p_r dr = n_r h$ and $\int p_\varphi d\varphi = kh$. However, Wentzel was unable to decide about the normalization of the action variables, so his method did not yield any information on whether the denominator in the Balmer expression was an integer or a half-integer. Wentzel also treated the relativistic Kepler problem and he arrived, in fact, to an energy expression which was formally identical to the exact Sommerfeld formula. However, Wentzel's theory could not be regarded as satisfactory: For one thing, the determination of the values of the quantum numbers was left undecided. And for another thing, the formal agreement with Sommerfeld's *exact* formula appeared to be rather fortitious: Wentzel's result was obtained as an approximation where terms, smaller than c^{-2}, were neglected, and also he did not take spin into account. Commenting on the early quantum mechanical attempts to deal with the hydrogen atom, Van Vleck has recalled: "The last days of the old quantum theory were the golden age of empiricism, where physicists often obtained correct answers by appropriate doctoring of formulas based on questionable theory, and some of this empiricism still survived in the very early days of quantum mechanics."[94]

This observation holds particularly well for the works reviewed in this chapter, and not least for Wentzel's theory.

That Wentzel's theory, despite of its derivation of a Sommerfeld formula, was not a satisfactory quantum mechanical answer to the fine-structure of hydrogen, was fairly evident. Schrödinger, who had worked on the same problem from his wave mechanics, was not impressed by the matrix physicists' laborious calculations on the hydrogen atom. In a letter to Lorentz he dismissed these attempts as being largely without scientific value, and being definitely inferior to his own, wave mechanical approach:

> "Dirac (Proc.Roy.Soc.) und Wentzel (Z.f.Phys.) rechnen Seiten lang am Wasserstoffatom, Wentzel auch relativistisch, wobei im Endresultat bloss das fehlt, was einen eigentlich interessiert: nähmlich, ob "halbzahlig" oder "ganzzahlig" zu quanteln ist! So findet Wentzel also zwar "genau die Sommerfeldsche Feinstrukturformel", aber aus dem angegebenen Grunde ist das Resultat für den Erfahrungsvergleich ganz Wertlos. In der Wellenmechanik ergibt die relativistische Behandlung, die ebenso einfach ist, wie die klassische, unzweideutig halbzahliges Azimuth- und Radialquant. (Ich habe die Rechnung seiner Zeit nicht publiziert, weil dies Ergebnis mir eben zeigte, dass noch etwas fehlt; dieses etwas ist sicher der Gedanke von Uhlenbeck und Goudsmidt.)"[95]

Also Pauli did not consider Wentzel's theory to be the proper relativistic quantum mechanics. In private letters, he objected to Wentzel's method.[96] In particular, Pauli pointed out that one had to take the spinning electron, now being acceptable after Thomas' theory (below), into account:

> "Meine Meinung ist also jetzt die, dass.... Ihr Resultat über die Sommerfeldsche Formel mit halbein [?] k, was die höheren Relativitätskorrektionen betrifft, physikalisch unzutreffend ist. Das ganze Problem ist wohl nur mit Berücksichtigung des Elektronen-Momentes vernünftig zu behandlen. (Das war, glaube ich,

auch Sommerfelds Meinung in Zürich).
Was ich erhoffe, ist, dass die Sommerfeldsche Formel (bei Berücksichtigung von Relativität und Elektronen-Moment) auch für die höheren Korrektionen sich streng aus vernünftigen theoretischen Ansätzen wird ableiten lassen (wobei natürlich j an Stelle von k treten muss). Dass aber bei Ausserauchtlassen des Elektronen-Momentes die Sommerfeldsche Formel in Bezug auf die höheren Korrektionen noch irgend einen Sinn behält, wenn mann in ihr die Zahl k halbzahlig setzt, glaube ich jetzt nicht mehr."[97]

That Pauli was much occupied with the problem of uniting quantum mechanics, spin and relativity in order to reproduce the fine-structure etc., is manifest from his correspondence, and from remarks in his papers. Pauli's occupation with this subject resulted in a critical insight in the problem.[98] In a footnote in Wentzel's paper it is stated, that Pauli had orally demonstrated how Sommerfeld's formula may be derived and that he had found that the quantum numbers are to be half-integers; this disagrees with Sommerfeld's formula, but may, according to Wentzel, be rectified if the spin hypothesis is taken into account.

As mentioned, it was a great release to the theoretical physicists of the time, when the 'riddle of the 2-factor' was eventually dissolved by Thomas in March 1926. From that time the spinning electron became an accepted part of quantum calculations, although its more intimate relationship to quantum mechanics was still obscure. Working in Bohr's institute in Copenhagen, L.H.Thomas from Cambridge subjected the kinematics of a spinning electron to a careful, relativistic analysis.[99] Thomas showed, that the 'riddle of the 2-factor' was in fact not based in any deficiency of quantum theory, but in an incomplete use of relativistic kinematics. By applying Lorentz transformations successively to the motion of the spinning electron, Thomas showed that it contributes to the energy with a spin-orbit coupling term of value

$$\frac{Ze^2}{2m^2c^2r^3}\,\vec{k}\cdot\vec{s} \qquad (4.2)$$

where $\vec{s}$ is the spin angular momentum. This was just half of the value previously calculated. With Thomas' result, the width of the spin doublets came out right. In an optimistic mood, reflecting the general feeling among quantum theorists, Kramers reported from Copenhagen:

> "I think that the great advantages and the rescue our of so many difficulties with the ideas of spinning electrons affords are exposed in that latter [i.e. Goudsmit's and Uhlenbeck's letter to *Nature*] in most convincing and physical way. A few days ago we had moreover an agreeable surprise, when Thomas from Cambridge, who is working here, found out of a most interesting error, which causes the difficulty that the spin doublets should be twice too large disappear. Since further Heisenberg and Pauli have succeeded in finding the quantum mechanical mean values of $[r^{-2}]$ and $[r^{-3}]$ for a Keplerian orbit, we know now that the fine structure theory of the hydrogen spectrum and the theory of the doublets in X-ray spectra is in finest order..."[100]

The next step to take was to apply the new insight to the theory of spectra, and in particular to the fine-structure of hydrogen. This step was immediately taken by Heisenberg and Jordan who, in March, considered the effects of spin and relativity.[101] These effects were treated as perturbations by means of the method developed in the famous 'Drei-Männer-Arbeit' some months before.[102] However, there is unpublished evidence that Heisenberg and Jordan had first attempted a more rigorous relativistic formulation in the hope that this would supply a quantum mechanical explanation of spin. The 9.th of December 1925 Heisenberg told Goudsmit:

> "Freilich glaub ich doch auch, dass die endgültige Lösung noch tiefer liegt und wesenlich mit einer vierdimensional-invarianten Formulierung der Quantenmechanik zu tun hat. Gegen die wörtliche Anwendung Ihrer Hypothese sprechen, glaub ich, doch manche Argumente. Erstens ist da dieser Faktor 2, der wirklich eine direkte Übere-

> instimmung mit der Erfahrung verhindert....
> Ich versuche hier jetzt mit Jordan eine vierdimensionale Formulierung der Quantenmechanik und bin neugierig, was dabei herauskommt."[103]

This ambitious project, only finished with Dirac's theory some two years later, had to be given up and was substituted with the more modest, but also more manageable and highly successful, theory of March 1926.

In February, Heisenberg reported to Goudsmit that he and Jordan had succeeded to take over the spin theory into matrix mechanics: "Die Rechnungen über Ihr Modell nach der Quantenmechanik sind jetzt abgeschlossen (z. Teil in Verein mit Pauli) und das Resultat ist in jeder Beziehung das erwartete."[104] For the doublet structure, however, Heisenberg communicated the result

$$H = H_0 + \frac{2R^2h^2Z^4}{mc^2n^3}\left(\frac{j(j+1)-k(k+1)-\frac{1}{2}\cdot\frac{3}{2}}{k(k+\frac{1}{2})(k+1)} - \frac{1}{k+\frac{1}{2}} + \frac{3}{4n}\right) \quad (4.3)$$

where the first term in the bracket is due to spin, the two latter to relativity (see also below). Heisenberg commented on this result:

> "Die Relativität gibt nichts die Sommerfeldsche Formel; bei Sommerfeld hiessen ja die letzten beiden Glieder der Klammer $\left(-\frac{1}{k+1}+\frac{3}{4n}\right)$. Also
>
> fällt jedenfalls die relativistische Erklärung der Dubletts fort. Aber weiter: Ihre Theorie gibt genau das doppelte, der beobachteten Feinstrukturaufspaltung. Daher ergibt sich auch keine Trennung in Abschirmungsdubletts und magnetische Dubletts. Aber es gibt die merkwürdige Beziehung: Würde man bei Ihren Elektron den Faktor 2 streichen, so ergäbe sich erstens die richtige Dublettgrösse, zweitens die richtige Trennung in Abschirmungs- und magnetische Dubletts; d.h. exakt die Sommerfeldsche Formel."[105]

As this letter shows, the Göttingen physicists were still haunted by the 'riddle of the 2-factor', which destroyed the otherwise so remarkable agreement with experience. The resolution of the riddle, Thomas' explanation, was offered only a few days after (Thomas' result may rather accurately be dated 20-24 February 1926, cf. Kramers' letter, above). When the news from Copenhagen reached Göttingen, Heisenberg and Jordan quickly corrected their results and submitted their paper for publication.

In their paper, Heisenberg and Jordan expressed the Hamiltonian for an atom in an external magnetic field, $\vec{H}$, as

$$H = H_0 + H_1 + H_2 + H_3$$

H_0 denotes the unperturbed energy levels, Bohr's result. The three correction terms are due to the magnetic field (H_1), the spin-orbit coupling (H_2) and the relativistic mass variability (H_3). The first term was immediately written as

$$H_1 = \vec{\mu}_{total} \cdot \vec{H} = \frac{e}{2mc}\vec{H} \cdot (\vec{k}+2\vec{s})$$

consisting of the magnetic energy of the orbital motion and the magnetic energy of the spinning electron. For H_2, Thomas' result was used, i.e. (4.2). The relativistic correction is given by (4.1). By means of perturbation theory, and by assuming the relations

$$\vec{s}^2 = s(s+1)\left(\frac{h}{2\pi}\right)^2, \text{ and } \vec{s}\times\vec{s} = -\frac{h}{2\pi i}\vec{s}$$

to hold by analogy with the properties of the orbital angular momentum $\vec{k}$, Heisenberg and Jordan were able to give a satisfactory explanation of the old quantum theory's doublet formulae and to derive Landé's g-value. Furthermore, the spectral intensities were calculated and turned out to be in good agreement with experience.

For the calculation of the H_2 and H_3 contributions, Heisenberg and Jordan were again faced with the problem which had troubled Pauli in his paper on the hydrogen atom, i.e. to evaluate the time averages of r^{-2}, and now also of r^{-3}, the latter from the Thomas term. Taking advantage of Pauli's analysis, Heisenberg and Jordan succeeded in calculating these mean values. In the case of no external magnetic field, their result for the perturbation energy was written

$$\Delta H = H_2+H_3 = \frac{2R^2h^2Z^4}{mc^2n^3}\left(\frac{j(j+1)-k(k+1)-s(s+1)}{2k(k+\frac{1}{2})(k+1)} - \frac{1}{k+\frac{1}{2}} + \frac{3}{4n}\right) \qquad (4.4)$$

This result differs from (4.3) only by the factor of one half in H_2, arising from the Thomas result. j is the quantum number for the compound angular momentum

$$\vec{j}^2 = j(j+1)\left(\frac{h}{2\pi}\right)^2 = (\vec{k}+\vec{s})^2$$

If now the spin quantum number s is put equal to $\frac{1}{2}$, and if k is replaced with $j\pm\frac{1}{2}$, the energy contribution becomes:

$$\Delta H = \frac{2R^2h^2Z^4}{mc^2n^3}\left(-\frac{1}{j+\frac{1}{2}} + \frac{3}{4n}\right)$$

This is the same as the reinterpreted (approximate) Sommerfeld formula, i.e. agreeing with the current knowledge of fine-structure (since j is half-integral, $j+\frac{1}{2}$ attains the same values as k).

Using a similar perturbation technique as Heisenberg and Jordan, but without knowing about their work, Richter at Caltech, USA, also found the energy correction due to combined spin and first order relativity effects.[106] Richter's results were the same as those of Heisenberg and Jordan.

In effect, with Heisenberg and Jordan's important contribution, matrix mechanics had accounted for the hydrogen spectrum in a highly satisfactory way. It was the first time the new mechanics reproduced the old 'relativistic' Sommerfeld formula, which was now, however, shown to be the result of a combination of spin and relativity. If there were still any sceptics as to the usefulness of quantum mechanics, they were now convinced, of this as well as of the reality of spin.

Still, the success of the Heisenberg-Jordan theory was only rendered possible because spin and relativity were added as perturbations. Spin was taken over from Uhlenbeck and Goudsmit's hypothesis with Thomas' correction, and thus it had still not been accounted for in terms of quantum mechanics. And for relativity, the new spectral theory was not properly relativistic, since only the electron's mass variability was added as an approximation of first order. From a standpoint of conceptual beauty and inner consistency, these two features were unsatisfactory and should be sought completed. The ultimate theory, it was felt in some quarters, ought to be able to account for spin without extra hypotheses and should, furthermore, be genuinely relativistic, i.e. Lorentz invariant. This programme was pursuited by a number of physicists in 1926-27, though largely confined to the quarters of wave mechanics. It was, of course, only completed in 1928 by Dirac.

With the exception of Pauli's theory, all the works here mentioned (Dirac's, Wentzel's, Heisenberg and Jordan's), were based on two-dimensional models of the hydrogen atom. In wave mechanics, it will be recalled, it is essential to work in three dimensions if the results are to come out right. The matrix physicists' free use of two-dimensional models were therefore objectionable to Schrödinger, and particularly so after he had demonstrated the mathematical equivalence between matrix and wave mechanics. In continuation of the afore-mentioned letter to Lorentz, Schrödinger explained this point:

> "-Nebenbei bemerkt, ist Wentzels Ansatz so beschaffen, dass wenn er bis zum Resultat vordränge, sein Resultat wahrscheinlich falsch sein würde (d.h. nicht die wahre Aussage der Theorie darstellen), weil er das Problem zweidimensional fasst statt dreidimensional. Das ist, wie ich in der zweiten Mitteilung, S.32, hervorhob, nicht erlaubt - und ist, bei der vollkommen mathematischen Aequivalenz der Wellenmechanik und der Göttinger Mechanik, sicher auch in der letzeren unerlaubt. Die Wellenmechanik lässt hierfür den Grund auch klar erkenne, denn eine Wellenbewegung in zwei Dimensionen ist selbstverständlich etwas ganz anderes als eine Wellenbewegung in Drei Dimensionen. Dagegen kann mann, soweit ich sehe, in der Göttinger Mechanik nicht recht erkennen, weshalb die Reduktion des Problems durch Verwendung eines Integrals verboten sein soll."[107]

Schrödinger's observation appears to present a paradox: How can matrix and wave mechanics, being completely equivalent theories, yield the same results for the hydrogen atom, when the former operates in only two dimensions? Schrödinger seems to have believed that this 'paradox' was due to serious shortcomings in the matrix mechanical methods, if not in the foundation of matrix mechanics itself. The matter appears only more confusing when we read, in a footnote to Heisenberg and Jordan's paper, that: "Die exakten Berechnungen der Mittelwerte [of r^{-1}, r^{-2} and r^{-3}] für den dreidimensionalen Fall sind von W.Pauli ausgeführt worden und geben dasselbe Resultat wie die obigen Rechnungen."[108]

It turns out, such as explained by Van Vleck[109] in an interesting essay, that the distinction between two- and threedimensional treatments of the Kepler motion is essential, but was not adequately recognised among matrix physicists. It was, to use Van Vleck's phrase, only due to "a happy combination of empiricism and intuition," that they managed to come up with the correct answers based on twodimensional reasoning. For it turns out, that rigorous calculations of the mean values of r^{-n} give in general other results than if applied to three dimensions. In general, Van Vleck shows, the correct calculation of passage from two to three dimensions is followed by replacing integral quantum numbers with half-integers. Thus, a correct calculation of (r^{-2}) and (r^{-3}) in two dimensions gives a formula for the energy correction which does not agree with experiment. But Heisenberg and Jordan found the "wrong" mean values for their twodimensional model, which happened to be the correct values for three dimensions. So the reason that two-dimensional matrix mechanical treatment of the hydrogen atom gives the right answer is due to a formal error of calculation. Schrödinger was, then, justified in expressing his doubts about the matrix physicists' use of two-dimensional models.

§ 5. SCHRÖDINGER'S WAYS TO THE WAVE EQUATION

When Schrödinger's wave mechanics was published, the formal core of the theory, the eigen-value wave equation, was derived in two, widely different ways. Both of these derivations were confined to the non-relativistic case.

The first published derivation, appearing on the first two pages of Q_1 (*Quantisierung ... Erste Mitteilung*), was not only curiously formal, but straightforwardly cryptical. On the whole this derivation appears badly justified, its sole foundation lying in its result, the eigen-value equation, and its successful application to the hydrogen atom. Anyhow, the essential content of Q_1 is not the derivation of the wave equation, but the equation itself and its mathematical treatment in order to solve the case of the hydrogen atom.

It is certainly not accidental that Schrödinger's first communication on wave mechanics starts right away with the hydrogen atom, and is in fact a new method to derive Bohr's old formula (3.1). If physicists were to be convinced about the soundness of the new wave mechanics, nothing better could be done than starting with the hydrogen atom. Just as in matrix mechanics (see § 4), the hydrogen atom was a test case also for wave mechanics. For Schrödinger, the hydrogen case played an important role not only in the 'context of justification' but, even more crucially, also in the 'context of discovery'.

In Q_2, the second communication on wave mechanics,[110] Schrödinger derived the wave equation in an alternative, and much better argued way. The core of the Q_2 derivation was an extension of Hamilton's old analogy between optics and mechanics. The approach taken by Schrödinger in Q_2 was adopted by virtually all contemporary commentators and was soon considered as *the* Schrödinger derivation of the wave equation. It is also this approach which most historians have suggested to be Schrödinger's original way to the wave equation. Indeed, Q_2 "could have preceded the first part from the logical point of view," such as remarked by Jammer.[111] This standard account of Schrödinger's making of wave mechanics finds a certain support in Schrödinger's monumental papers themselves. Already in Q_1 Schrödinger recognized, for instance, the unsatisfactory, non-intuitive and *ad hoc* character of the first derivation. The formal introduction of the ψ function, Schrödinger explained, was to be related to a vibration process of some sort in the atom: "Ich hatte auch ursprünglich die Absicht, die neue Fassung der Quantenvorschrift in dieser mehr anschaulichen Art zu begründen, habe aber dann die obige neutral mathematische Form vorgezogen."[112] This 'intuitive' justification of the wave equation is, in the standard account, assumed to be the one which shortly after appeared in Q_2. In his second communication Schrödinger further emphasized the provisional character of the Q_1 method, which he now called "die an sich unverständliche Transformation [i.e. $S = K \ln \psi$] und den ebenso unverständlichen Übergang von der *Nullsetzung* eines Ausdrucks zu der Forderung, dass der *Raumintegral* des nämlichen Ausdruckes *stationär* sein soll."[113] The Q_1 approach, Schrödinger continued, "sollte nur zur vorläufigen raschen Orientierung über den äusserlichen Zusammenhang zwischen der Wellengleichung und der H.P. [Hamilton's partial differential equation] dienen."[114]

There are good reasons, however, to agree with Wessels[115] when she argues that Q_2 was not Schrödinger's original way to wave mechanics, but that Q_2 came after Q_1 not only chronologically but also genetically. Science does not always progress in accordance with logic. That Schrödinger's published presentation of his ideas accords with the order in which these ideas were fostered, is actually what we are told by Schrödinger himself. In November 1926, he emphasized in the preface to the book edition of his papers on wave mechanics that "die hier zu einem Bändchen vereinigten Arbeiten *nacheinander* entstanden sind. Die Erkenntnisse spätere Abschnitte waren dem Schreiber der früheren häufig noch unbekannt."[116] While Hermann previously adopted the standard account,[117] he has later changed his view in accordance with Wessels': The basis of wave mechanics, including the Schrödinger equation, was worked out before Schrödinger turned to the Q_2 approach. According to Hermann, it was only in February 1926 that Schrödinger became acquainted with Hamilton's mechanical-optical analogy.[118]

I agree with Wessels that Q_1 was prior to Q_2. But even if the detailed Q_2 approach was unknown to Schrödinger in January 1926, the general argumentation of Q_2, i.e. that the new wave mechanics relates to geometrical optics, was most probably in Schrödinger's mind also at that time. The idea of reconstructing mechanics in analogy with a generalized optics, following Hamilton's original ideas, had not only been highlighted by Felix Klein[119] (who did not, of course, consider the connection to quantum theory). But, more important, de Broglie had made extensive use of the analogy between optics and mechanics (see § 1), although not in Hamilton's sense, which was apparently unknown to de Broglie (on the whole, Hamilton's works were not widely known on the Continent). Actually, Schrödinger's concern with Hamiltonian mechanics and optics was of an elder date. Some years before wave mechanics, he had thoroughly investigated Hamilton's optical-mechanical analogy as well as other subjects from analytical mechanics which happened to be useful in his later exposition of wave mechanics. This is shown by the content of Schrödinger's notebooks on "Tensoranalytische Mechanik" from 1918-1922,[120] in which Schrödinger closely examined the mechanical analogy to optics and its relation to the Hamilton-Jacoby equation. So it is a small wonder that Schrödinger recalled this analogy and its relevance to his wave mechanical programme at an early stage of his investigations. In fact, in one of Schrödinger's earliest research notebooks on wave mechanics,[121] written in December 1925 or early January 1926, he explicitly refers to "Die alte Hamiltonsche Analogie zwischen Optik u. Mechanik", in order to apply it to his new ideas. At this occasion, Schrödinger derived the wave equation in the same manner as he did in Q_2 but was not able to find the energy spectrum from the radial part of the equation.

Anyway, Hermann's assertion that Schrödinger did not know about the Q_2 approach until February 1926 is completely wrong. Even if it is not mentioned in the text itself, some kind of optical-mechanical considerations probably played a part also in Schrödinger's first communication. These considerations, however, have hardly been Hamilton's analogy itself; rather, it was an optical theory due to Debye, Sommerfeld and Runge which at this stage served as an inspiration to Schrödinger.

In Q_1 Schrödinger started from the general H.J. (Hamilton-Jacobi) theory of macro-mechanics, according to which the integral of the equation of motion is of the form

$$H\left(q_k, \frac{\partial S}{\partial q_k}\right) = E \qquad (5.1)$$

Here, S is the so-called Hamilton's characteristic function. The action function S relates to the momenta by

$$p_k = \frac{\partial S}{\partial q_k} \qquad (5.2)$$

The energy of a single particle moving in an electrostatic field is

$$E = \frac{1}{2m}(p_x{}^2+p_y{}^2+p_z{}^2) + U \qquad (5.3)$$

where $U = -e^2/r$. In H.J. formulation the energy expression gives

$$\left(\frac{\partial S}{\partial x}\right)^2 + \left(\frac{\partial S}{\partial y}\right)^2 + \left(\frac{\partial S}{\partial z}\right)^2 = 2m(E-U)$$

which may also be written

$$(\nabla S)^2 = 2m(E-U) \qquad (5.4)$$

In Q_1 Schrödinger immediately, and without any explanation, replaced S in (5.1) by the substitution

$$S = K \ln \psi \qquad (5.5)$$

K is an unknown constant with dimension of an action, to be determined in the course of further investigation (where it turns out to be $^h/2\pi$). The famous ψ, here appearing for the very first time, is prosaically referred to as just "eine neue unbekannte."

Why did Schrödinger apply the "unverständliche Transformation" (5.5) ? Kubli[122] has argued that the cryptical replacement of S with $\ell n\psi$ was suggested to Schrödinger from optical theory. Let us develop Kubli's suggestion a little closer. If one shall pass from macro-mechanics, eq. (5.1), to a new appropriate micro-mechanics - and that was Schrödinger's idea - then the connection between geometrical and wave optics may serve as a valuable guide. This connection had been exposed in 1911 by Sommerfeld and Runge,[123] who developed some of the ideas due to Hamilton. Sommerfeld and Runge's work was, as they reported in their paper, indebted to an oral communication from Debye. It is natural to assume that Debye has drawn Schrödinger's attention to this old work from optics during one of the joint Zürich colloquia. The core of the Debye-Sommerfeld-Runge theory may be exposed as follows:

In wave optics, the basic equation is the well-known space form of the wave equation:

$$\Delta\psi + k^2\psi = o \qquad (5.6)$$

where $k = {}^{2\pi}/\lambda = nk_0$, k being the wave number and n the refractive index. In geometrical optics, on the other hand, the characteristic equation is the less well known *eikonal* equation:

$$(\nabla S)^2 = n^2 \qquad (5.7)$$

In the theory of eikonals, introduced by the astronomer H. Bruns in 1895, S = constant signifies a system of wave surfaces, corresponding to constant phases. The rays are directed along the normals of the S surfaces. The eikonal function S expresses, furthermore, the so-called optical length:

$$S_B - S_A = \int_A^B n \, ds$$

Indeed, the simplest solution to (5.7) is

$$S = n(\alpha x + \beta y + \gamma z) \quad \text{with} \quad \alpha^2+\beta^2+\gamma^2 = 1 \qquad (5.8)$$

In the Debye-Sommerfeld-Runge theory it was now demonstrated that the eikonal equation may be derived as a limiting case, $k\to\infty$ or $\lambda\to o$, of the wave equation. In (5.6) the planewave solution is

$$\psi = Ae^{ik(\alpha x+\beta y+\gamma z)}$$

Recalling the interpretation of S as an optical length, (5.8), one put

$$\psi = Ae^{i\frac{k}{n}S} \qquad (5.9)$$

Here, A is considered to be a 'slowly' varying quantity (viz. compared to the rapid variation of ψ for $k\to\infty$). Calculation of $\Delta\psi$ with the approach (5.9) and insertion in (5.6) yields

$$[2i\frac{k}{n}(\vec{\nabla}S\cdot\vec{\nabla}A) + \Delta A+i\frac{k}{n}A\Delta S - \frac{k^2}{n^2}A(\nabla S)^2+k^2A]e^{i\frac{k}{n}S} = o$$

For large k (geometrical optics) the first three terms may be cancelled. What remains is the eikonal equation. I.e., geometrical optics has been derived as a limiting case of wave optics.

In Schrödinger's programme a kind of reversed trend was followed, since he tried to formulate an undulatory mechanics, related to ordinary macro-mechanics in the same way as wave optics relates to geometrical optics. To pass from ordinary mechanics to wave mechanics would then mean to apply the reverse of the transformation (5.9) to the H.J. equation, the Hamiltonian function S now being interpreted as the eikonal S. From (5.1) follows that in the wave picture, S is expressed by $K\ell n\psi$, such as used by Schrödinger in Q_1.

To which extent this kind of argumentation played a role for Schrödinger's approach in Q_1 is unknown. There is no hard evidence for the impact of the Debye-Sommerfeld-Runge theory on Schrödinger's thinking. It was only in Q_2 that Schrödinger referred to it, and then without mentioning the eikonal by name.[124]

Returning to the content of Q_1, the substitution (5.5) leaves now the H.J. equation in the form

$$H(q_k, \frac{k}{\psi}\frac{\partial\psi}{\partial q_k}) = E$$

or, from (5.3)

$$(\nabla\psi)^2 - \frac{2m}{K^2}(E-U)\psi^2 = o \qquad (5.10)$$

In Q_1 Schrödinger now took as his fundamental equation, not (5.10) itself but the one resulting from a variational procedure, viz. that the integral of the quadratic form in ψ and $\partial\psi/\partial q$ in (5.10) shall be stationary:

$$\delta\int[(\nabla\psi)^2 - \frac{2m}{K^2}(E-U)\psi^2]dq = o \qquad (5.11)$$

From the calculus of variation it is known that the above problem may be transformed to a differential equation by means of the so called Euler-Lagrange conditions. Using Cartesian coordinates, dq = dxdydz, the differential equation turns out to be

$$\Delta\psi + \frac{2m}{K^2}(E-U)\psi = o \qquad (5.12)$$

i.e. the Schrödinger equation (still with $U = -e^2/r$).

While the formulation of (5.5) may be explained as a transformation of the mechanical equation of motion into a wave picture, guided by the Debye-Sommerfeld-Runge theory, the application of the variational procedure ("den ebenso unverständlichen Übergang...") still lacks justification beyond that it results in a useful equation. On the other hand, it was in 1925 well known that all physical laws, in the classical as well as in the relativistic domain, can be formulated by some variational principle; most physicists, probably, shared Planck's credo that "the principle of least action.... appears to govern all reversible processes in Nature."[125] So the idea to obtain the wave mechanical law by means of a variational principle was not unnatural. Also it may have appealed to Schrödinger, who conceived his new mechanics in a n-dimensional configuration space, that variational principles are independent of the special choice of coordinates. According to the memoir of Erwin Fues, at the time Schrödinger's assistant, the idea to deduce the wave mechanical equation by means of a variational principle was suggested by Debye in another of the Zürich colloquia, held in the beginning of 1926 (after 9 January, when Schrödinger returned to Zürich). Fues recalled that Debye's

> "Anregung erfolgte in einer Kolloquiumdiskussion nachdem Schrödinger seine unrelativistische Theorie vorgetragen hatte. Soviel ich mich erinnere, sagte Debye (dem Sinne nach, nicht mit diesen Worten) nur, dass es gelungen sei, den wichtigsten grundlegenden Theorien in der Physik die Form eines Variationsprinzips zu geben, die eine eindrucksvolle Zusammenfassung sei."[126]

Anyway, when Schrödinger applied the variational procedure of Q_1 in January 1926, he knew beforehand what to look for. An examination of Schrödinger's notebooks[127] testifies that he only applied the Q_1 method after he had found a candidate for the differential equation, sought for, by means of a direct use of de Broglie's formulae (see §8). This candidate he had tried to solve, i.e. to find its energy spectrum, but had failed because of mathematical difficulties. The fact that Schrödinger knew the result before he engaged in the Q_1 derivation, explains the *ad hoc* character of this first published derivation.

It should be remarked, that although Schrödinger in Q_1 did only consider non-relativistic mechanics, his chosen method is perfectly applicable also in the relativity case. We only have to replace (5.3) with the corresponding relativistic energy expression, which then gives the relativistic H.J. equation

$$(\nabla S)^2 = \frac{1}{c^2}(E-U)^2 - m_0^2 c^2 \qquad (5.13)$$

This replaces (5.4), the only difference being that E now denotes the total energy, including $m_0 c^2$. Following the procedure outlined above, the variational principle becomes

$$\delta \int \{(\nabla\psi)^2 - \frac{1}{K^2 c^2}[(E-U)^2 + m_0^2 c^4]\psi^2\} dq = o$$

The corresponding differential equation is the relativistic Schrödinger equation, also known as the Klein-Gordon equation (see §§8,11). A similar result was obtained by Schrödinger in early January 1926. At this occasion (we are referring to his notebooks) he also considered another version of the Q_1 method. The substitution (5.5) was written as

$$S = iK \ln \psi \quad \text{or} \quad \psi = e^{-i\frac{S}{K}}$$

Schrödinger now tries to consider only the imaginary part of

$$e^{i\frac{S}{K}} = \cos(\frac{S}{K}) + i\sin(\frac{S}{K})$$

that is, he substitutes S with

$$S = K \arcsin \psi \tag{5.14}$$

This substitution applied to the relativistic H.J. equation (5.13) gives

$$(\nabla\psi)^2 - \frac{1}{K^2c^2}[(E-U)^2 + m_0^2c^4]\cdot(1-\psi^2) = 0$$

By applying the variational principle to this equation, Schrödinger arrives at

$$\Delta\psi - \frac{m_0^2c^2}{K^2}\left[\left(\frac{m_0c^2}{E-U}\right)^2 - 1\right]\psi = 0 \tag{5.15}$$

being another candidate for the (relativistic) wave equation. Schrödinger apparently had hoped that (5.15) would lead to a mathematically more manageable differential equation than his first candidate. However, (5.15) is not simple, and after a half-hearted attempt to determine its energy spectrum, Schrödinger leaves it.

We shall now proceed to Schrödinger's derivation of the wave equation such as presented in his second communication. The Q_2 approach has often been analyzed in depth, technically as well as historically.[128] Since we are here mainly concerned with the original creation of the Schrödinger equation, and since the Q_2 method was only third in the row of derivations, we shall suffice to outline a highly condensed version of Schrödinger's very detailed arguments in Q_2.

In classical Hamiltonian theory the basic equation is

$$\frac{\partial W}{\partial t} + T(q_k, \frac{\partial W}{\partial q_k}) + U(q_k) = 0 \tag{5.16}$$

Here W is Hamilton's principal function, given by $\int(T-U)\,dt$; T is the kinetic energy. W relates to the

action function S, used above, by

$$W = S - Et$$

From (5.3) the H.J. equation may be written[129]

$$(\nabla W)^2 = 2m(E-U) \qquad (5.17)$$

This is virtually the same as (5.4), due to $p_k = \frac{\partial W}{\partial q_k} = \frac{\partial S}{\partial q_k}$

Following Hamilton, Schrödinger considered the system of W-surfaces for which W = constant, as a system of wave surfaces due to a progressive, but standing wave in the configuration space. The velocity of the system is perpendicular to the surfaces of W = constant, a result derived from $\vec{p} = \nabla W$. In the time interval dt the system moves the normal distance

$$ds = \frac{dW}{\sqrt{2m(E-U)}}$$

such as obtained from (5.17). Since $E = {}^{dW}/dt$ this may also be written

$$ds = \frac{E\,dt}{\sqrt{2m(E-U)}}$$

The velocity of propagation of the W-surfaces is then

$$V = \frac{ds}{dt} = \frac{E}{\sqrt{2m(E-U)}} \qquad (5.18)$$

Since W in the geometric wave system plays the role of a phase, V is a phase velocity. It is different from the particle velocity, which is $\sqrt{^2/m(E-U)}$.

Up to this point Schrödinger's work was nothing but a slightly different way of presenting Hamilton's old theory. To construct a wave equation, he had to provide the W-phases with a frequency. This was done by assuming the validity of the Planck-Einstein relation, i.e. by putting

$$\nu = {}^{E}/h$$

That is

$$V = \frac{h\nu}{\sqrt{2m(h\nu - U)}} \tag{5.19}$$

Schrödinger assumed that his ψ waves travelled with the W-waves and that their equation was the usual second-order differential equation

$$\Delta\psi - \frac{1}{V^2}\frac{\partial^2\psi}{\partial t^2} = o \tag{5.20}$$

Finally, by the natural assumption of sinusoidal time dependency

$$\psi(q,t) = \psi(q)e^{2\pi i\nu t} = \psi(q)e^{i\frac{2\pi}{h}Et} \tag{5.21}$$

and by introducing (5.18), the time-independent Schrödinger equation (5.12) comes out.

As with the Q_1 method, Schrödinger's non-relativistic Q_2 method may easily include relativity (which Schrödinger did not do in Q_2). By virtue of (5.13) the relativistic phase velocity now becomes

$$V = \frac{hc\nu}{\sqrt{(E-U)^2 - m_0^2c^4}}$$

If inserted in the usual wave equation, this gives again the Klein-Gordon equation.

One of the reasons to the standard account of the genesis of wave mechanics, i.e. that Q_2 was worked out before Q_1, is, no doubt, that the Q_2 approach relies very much on de Broglie's theory while the Q_1 approach does not.

Apparently the Q_1 method has nothing whatsoever to do with de Broglie's phase waves. On the other hand, the approach taken in Q_2 is clearly inspired by de Broglie. Schrödinger acknowledged his debt to de Broglie's "schönen Untersuchungen welchen ich die Anregung zu dieser Arbeit verdanke."[130] The wavelength of Schrödinger's waves may be got from (5.19) and is

$$\lambda = \frac{V}{\nu} = \frac{h}{\sqrt{2m(E-U)}}$$

this is, of course, nothing else than de Broglie's famous $\lambda = h/p$ formula.

With some justification, Schrödinger may be attributed also a third (or rather a fourth) approach to his wave equation. This is based on the substitutions

$$E \rightarrow \frac{ih}{2\pi}\frac{\partial}{\partial t}, \qquad P_k \rightarrow \frac{h}{2\pi i}\frac{\partial}{\partial q_k} \tag{5.22}$$

which soon became the standard procedure for obtaining formulae in quantum mechanics. In Schrödinger's intervening paper on the equivalence between matrix and wave mechanics,[131] he had taken the step to represent the momenta p_k with the differential operators given by (5.22). However, he did not at that stage apply the procedure also to the energy equation in order to obtain an operator formalism for the energy. As mentioned (§ 2), this was done by Born and Wiener even before wave mechanics had appeared;[132] but Born and Wiener did not extend their energy operator presentation to cover also an operator formalism for the momenta. It was only in Schrödinger's fourth communication on wave mechanics,[133] Q_4, that he considered a proper operator prescription, and then in order to obtain the relativistic wave equation (see § 6). In Q_4 Schrödinger proposed to derive the wave equation from the Hamilton-Jacobi equation by means of the substitutions

$$\frac{\partial W}{\partial t} \to \pm \frac{h}{2\pi i} \frac{\partial}{\partial t}, \qquad \frac{\partial W}{\partial q_k} \to \pm \frac{h}{2\pi i} \frac{\partial}{\partial q_k} \tag{5.23}$$

Apart from the double signs (which Schrödinger used to account also for the complex-conjugate time-dependent equation), this is the same as (5.22). Schrödinger emphasized in Q_4 that this prescription was a "*rein formale* verfahren", justified only by the fact that the non-relativistic equations

$$\left(-\frac{h^2}{8\pi^2 m}\Delta + U\right)\psi = \pm \frac{h}{2\pi i}\frac{\partial\psi}{\partial t}$$

may in this way be obtained from the classical equation (5.3). Schrödinger's operator prescription is, however, a product of quantum mechanics, not an original means to derive the equations of wave mechanics. In the genesis of the Schrödinger equation, this method played no role.

§ 6. RELATIVITY IN SCHRÖDINGER'S WORK

As we have seen, the really important (or, anyway, the really convincing) thing in Schrödinger's first paper on wave mechanics was the derivation of Bohr's formula for the energy levels of hydrogen. Bohr's principal quantum number, n, was there introduced as an index in the mathematical function used to solve the eigen-value equation. This appearance of n, from mathematical analysis and not from the postulates of the old quantum theory, was a highly satisfying feature to Schrödinger. On the very first lines of Q_1, he stressed how his theory gives "die Ganzzahligkeit auf dieselbe natürliche Art, wie etwa die Ganzzahligkeit der *Knotenzahl* einer schwingenden Saite."[134] And later in Q_1 he assessed the merits of his theory so far:

> "Als das wesentliche erscheint mir, dass in der Quantenvorschrift nicht mehr die geheimnisvolle 'Ganzzahligkeitsvorderung' auftritt, sondern diese ist sozusagen einen Schritt weiter zurückverfolgt: sie hat ihren Grund in der endlichkeit und Eindeutigkeit einer gewissen Raumfunktion."[135]

To Schrödinger the wave mechanical theory's nearness to classical concepts as well as its familiar methods of classical mathematical analysis, was a very qualifying feature, so as it was for many members of the physical community of the time. This formal familiarity was particularly distinct when compared to the Göttingen quantum mechanics, which made Schrödinger "durch den Mangel an Anschaulichkeit abgeschrecht, um nicht zu sagen abgestossen."[136] Like many of his colleagues, Schrödinger deeply disliked the Göttingen *Atomystik*.[137] His whole research programme was directed towards a rehabilitation of the methods and concepts of classical physics, particularly its continuum aspects.[138] In February 1926 he thus told Planck:

> "Ich habe die allerverwegensten Hoffnungen, dass es jetzt gelingen wird, eine harmonische, von allen Härten freie Quantentheorie aufzubauen und zwar nicht in dem Sinne, dass alles immer unstetiger und ganzzahliger wird, sondern gerade im umgekehrten Sinn: die schönen klassischen Methoden liefern selbstätig alle Ganzzahlighkeit, die man braucht, es ist keine Mystik in den ganze Zahlen, es sind die nähmlichen, die uns in Kugelflächenfunktionen, Hermite'schen und Laguerre'schen Polynomen (erstere beim Oszillator, letztere beim Wasserstoffelektron) längst vertraut sind. Sommerfelds Vergleich mit der Zahlenmystik der Pythagoräer stimmt genau: die Ganzzahligkeiten im Atom haben ungefär denselben Grund wie die harmonischen Obertöne einer schwingenden Saite."[139]

Aesthetic and extra-scientific considerations admittedly played a great role for Schrödinger in his creation of physics, such as pointed out by Scott and by Raman and Forman. It is true, that Schrödinger loathed matrix mechanics' lack of *Anschaulichkeit* and that his general, aesthetic aversion against Heisenberg's approach determined a large part of Schrödinger's research programme from 1926 onwards. From Schrödinger's philosophic standpoint, he was bound to be strongly opposed to the Göttingen mechanics such as it emerged in the autumn of 1925. But from this, to claim that "a sense of aesthetics inspired him to formulate the wave mechanics,"[140] is grossly to overstate the point. Schrödinger's aesthetic feelings played, in 1925, a negative role in preventing him from accepting matrix mechanics; they did not positively cause him to embark upon his wave mechanical 'alternative' (in the creative phase, December 1925, Schrödinger did not conceive his new ideas as an alternative to matrix mechanics). Also, Schrödinger's philosophical and aesthetic emotions were, undoubtedly, active in his sympathy to de Broglie's work; but in 1925, de Broglie's theory was, largely, considered unconnected with the new quantum mechanics of Göttingen and Cambridge.

Schrödinger's wave mechanics had its background in de Broglie's theory which was (cf. § 1) thoroughly relativistic. In regard of this it may seem strange that the original wave mechanics appeared in a non-relativistic form. This peculiarity was clearly recognized by Schrödinger. In the autumn of 1926, Schrödinger ended a review of his theory, written for an American audience, in this way:

> "... the undulatory theory of mechanics has been developed without references to two very important things, viz. (1) the relativity modifications of classical mechanics, (2) the action

> of a magnetic field on the atom. This may be thought rather peculiar since L. de Broglie, whose fundamental researches gave origin to the present theory, even started from the relativistic theory of electronic motion and from the beginning took into account a magnetic field as well as an electric one."[141]

The peculiarity pointed out by Schrödinger turns out to be tightly connected with the way in which wave mechanics was borned. In fact, Schrödinger started his investigations on an undulatory mechanics with a relativistic attempt which was never published. Before we examine Schrödinger's early work on relativistic wave mechanics, we shall consider the matter as may be glimpsed from the published articles.

In Q_1 Schrödinger directly expressed his awareness that the non-relativistic treatment was not entirely satisfying. Schrödinger was afraid that his new ideas might "in ihren Ergebnissen ein blosser Abklatsch derüblichen Quantentheorie sein wird. Z.B. fürht das relativistische Keplerproblem, wenn man es genau nach der eingangs gegebenen Vorschrift durchrechnet, merkwürdigerweise auf *halbzahlige Teil*quanten (Radial- und Azimuthquant."[142] This interesting remark will be further discussed in the following, together with other evidences for an early relativistic theory.

In Q_1 Schrödinger also touched the relativity question in a rather cryptical passage on the relationship between the energy-eigenvalues E and the frequency ν of the corresponding eigenvibration.[143] In Q_2 this relationship was, in accordance with de Broglie's theory, shown to be $E=h\nu$, such as expected from quantum theory; his discussion of the $E-\nu$ relationship in Q_1 was there dismissed as being "einer blossen Spekulation."[144] But even if the Q_1 discussion is premature and perhaps speculative, it may be of some historical interest to deal with it; not only because it gives some hints to Schrödinger's early relativistic considerations but also because it provides a clue to the historical reconstruction of wave mechanics.

Schrödinger pointed out a contradiction between the expectations of quantum theory and of wave theory: While the first one demands a relation of the form $E \sim \nu$, the latter leads one to expect that $E \sim \nu^2$. This contradiction can be avoided, Schrödinger argued, if the E in the wave conception is taken to be the (negative) energy, appearing in Bohr's formula, plus a large constant C (which is assumed to be the electron's rest energy m_0c^2). Then $(E+C) \sim \nu^2$ and since $C \gg E$ the frequency of the vibration process may be expressed as

$$\nu = C'\sqrt{C+E} = C'\sqrt{C} + \frac{C'}{2\sqrt{C}} E + \ldots$$

This is in approximate agreement with "das "natürliche gefühl" des Quantentheoretikers... solange das Nullniveau der *Energie* nicht festgelegt ist." This idea also provides a wave mechanical understanding of Bohr's frequency condition (i.e. of $E'-E'' = h\nu$). On the other hand, Schrödinger points out, the Bohr relation is supposed to hold strictly while it gets only an approximate validity on this basis. But this disagreement is, according to Schrödinger, avoided if relativity is taken into account:

> "Das [i.e. the approximate character of the Bohr relation] ist aber nur scheinbar und wird völlig vermieden, wenn man die *relativistische* Theorie entwickelt, durch welche überhaupt erst ein tieferes Verständnis vermittelt wird. Die grosse additive Konstante C hängt natürlich aufs innigsten zusammen mit der Ruhenergie mc^2 des Elektrons. Auch das scheinbar *nochmalige* und *unabhängige* Auftreten der Konstante h.... in der Frequenzbedingung wird durch die relativistische Theorie aufgeklärt bzw. vermieden. Aber leider begegnet ihre einwandfreie Durchführung vorläufig noch gewissen, oben berürhten Schwierigkeiten."

Why and how a relativistic wave mechanics may save the mentioned disagreement is not explained by Schrödinger.

Although Schrödinger was most aware of the difficulties which the non-relativistic form of his theory implied, he had in early 1926 great confidence in his undulatory approach and he felt sure that it could be generalized to include not only relativity but also spin without destroying its results obtained on the non-relativistic basis. This confidence was expressed in print as well as in private letters.[145] In the spring of 1926 Schrödinger's confidence seemed justified by the many results so brilliantly achieved by the non-relativistic theory: apart from the derivation of Bohrs formula for the hydrogen atom, Schrödinger had successfully applied his methods to such problems as the harmonic oscillator, rigid and nonrigid rotator, Stark effect (which, together with the hydrogen case, were the highlights of the applications), dispersion and selection rules for spectral transitions. These applications, together with the demonstration of equivalence between wave mechanics and matrix mechanics, left little doubt about the essential correctness of the theory.

It is, on the other hand, clear from Schrödinger's writings that he was constantly occupied with the lack of relativistic agreement and that he repeatedly tried to incorporate relativity in a satisfactory manner. Schrödinger realised, so as did other physicists (see § 4), that the problem of relativity was closely related to the problem of a satisfactory explanation of the anomalous Zeeman effect. It was in 1926 generally recognized that such an explanation was to rest on the spin theory. In this year, and the following, many physicists tried to work out quantum theories which could embrace spin and relativity at the same time.[146] In Q_1 Schrödinger did not mention spin, but latest in the spring of 1926 he had studied Uhlenbeck and Goudsmit's papers as well as those of Thomas and of Sommerfeld und Unsöld (see § 4), and he had also discussed the spin hypothesis with Pauli in Copenhagen and with Langevin in Paris. Schrödinger now felt that an interpretation of spin in terms of wave mechanics was contingent and would somehow solve his relativistic troubles. In Q_3 he wrote:

> "Diese [i.e. the Zeeman effect] erscheint mir unlöslich geknüpft an eine korrekte Formulierung des *relativistichen* Problems in der Sprache der Wellenmechanik, weil bei vierdimensionaler Formulierung das vektorpotential von selbst ebenbürtig an die Seite tritt....
> Man wird versuchen müssen den Uhlenbeck-Goudsmitschen Gedanken in die Wellenmechanik aufzunehmen."[147]

Schrödinger's remark about the four-dimensional formulation of wave mechanics was also stated in a footnote in Q_2.[148]

The relativistic Hamilton-Jacobi equation for an electron in an electromagnetic field may be written

$$\left(\frac{1}{c}\frac{\partial W}{\partial t} + \frac{e}{c}\varphi\right)^2 - \sum_{k=1}^{3}\left(\frac{\partial W}{\partial q_k} - \frac{e}{c}A_k\right)^2 = m_0^2c^2 \qquad (6.1)$$

or, by use of four-dimensional notation

$$(\nabla_\mu W - \frac{e}{c}\varphi_\mu)^2 = - m_0^2c^2$$

where $\varphi_\mu = (A_x, A_y, A_z, i\varphi)$ is the electromagnetic four-potential and ∇_μ is the four-dimensional gradient. These equations were included in Schrödinger's rough draft to Q_2.[149] According to Schrödinger, a wave mechanical translation of (6.1) runs into troubles, not met in the non-relativistic and non-magnetic case. Exactly which difficulties Schrödinger refers to, is not clear. As mentioned in the previous section, Schrödinger carried out the translation only in June, in his fourth communication.

In his paper on the relationship between matrix and wave mechanics, Schrödinger had ended with a suggestion about the representation of electrical charge density in wave mechanics. The charge density was there expressed as

$$\rho \sim \mathrm{Re}\,(\psi \frac{\partial \psi^*}{\partial t}) \qquad (6.2)$$

But shortly after,[150] Schrödinger realized this to be a failure and replaced it with

$$\rho \sim \psi\psi^*$$

The former expression, Schrödinger now stated, was introduced "durch das ich die spätere relativistische Verallgemeinerung zu erleichtern hoffte."[151] Again it is difficult to see exactly what Schrödinger means. However, since (6.2) has a striking similarity with the charge density appearing in relativistic quantum mechanics,[152] it may indicate Schrödinger's candidate for a relativistic charge density at the time.

It was only in Q_4 that Schrödinger took up a more detailed examination of the relativistic formulation of wave mechanics, and even then "nur mit der allergrössten Reserve."[153] To obtain the relativistic equation, Schrödinger now used the operator prescription, described in § 5. If applying this procedure to the Hamilton-Jacobi equation (6.1), the result becomes:

$$\Delta\psi - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \frac{4\pi i e}{hc}\left(\frac{\varphi}{c}\frac{\partial\psi}{\partial t} + \vec{A}\cdot\nabla\psi\right) + \frac{4\pi^2 e^2}{h^2 c^2}\left(\varphi^2 - \vec{A}^2 - \frac{m_0^2 c^4}{e^2}\right)\psi = 0 \qquad (6.3)$$

To get (6.3) from (6.1), one has to take advantage of the so-called Lorentz gauge in electrodynamics, viz.

$$\frac{1}{c}\frac{\partial\varphi}{\partial t} + \nabla\cdot\vec{A} = 0$$

Eq. (6.3) is, with Schrödinger's words, "die vermutete relativistisch-magnetische Verallgemeinerung" of the wave mechanical equation. When Schrödinger hesitatingly introduced the relativistic generalization in Q_4 he expressed his reasons to his "allergrösste Reserve" in two points: The one was of course the wrong fine-structure splitting, resulting from the corresponding eigenvalue equation; the other was that "die Verallgemeinerung beruht vorläufig auf rein formaler Analogie." In Q_4 Schrödinger did not elaborate any further on this equation and he did not attempt to investigate its physical content. He stated - but in words only - that he had applied the relativistic equation to the normal Zeeman effect and to rules of selection and polarization with the same result as in the non-relativistic case (an agreement which was obtained by neglecting the small $\vec{A}^2$ term). But what troubled Schrödinger and caused his lack of confidence in the relativistic approach, was its failure to account for the hydrogen spectrum. Considering this defect, eq.(6.3) could not be regarded to be satisfying.

Although Schrödinger's treatment of the relativistic wave equation in Q_4 stopped rather abruptly with (6.3), it may, for the sake of the further discussion, be useful to develop it into other forms. In the case of the hydrogen atom, not subject to an external magnetic field, we get

$$\Delta\psi - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} + \frac{4\pi i e^2}{hc^2 r}\frac{\partial\psi}{\partial t} + \frac{4e^2\pi^2}{h^2c^2}\left(\frac{e^2}{r^2} - \frac{m_0^2c^4}{e^2}\right)\psi = o \qquad (6.4)$$

For a free electron ($r\to\infty$) this reduces to

$$\left\{ \Delta\psi - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} + \left(\frac{2\pi m_0 c}{h}\right)^2 \right\}\psi = o \qquad (6.5)$$

To obtain the eigenvalue equation, $\psi(\vec{r},t)$ is substituted with the time-periodic $\psi(\vec{r})\exp(\frac{2\pi i}{h}Et)$. Then

$$\Delta\psi + \frac{4\pi^2}{h^2c^2}\left[\left(E + \frac{e^2}{r}\right)^2 - m_0^2c^4\right]\psi = 0 \qquad (6.6)$$

This equation is the relativistic counterpart to Schrödinger's eigenvalue equation (5.12), and the one which Schrödinger implicitly referred to in the beginning of Q_1.

§ 7. SCHRÖDINGER'S EARLY RELATIVISTIC QUANTUM MECHANICS: HISTORICAL EVIDENCES

We shall now consider the evidences in favour of the claim that Schrödinger had already worked out the foundations of a relativistic wave mechanics in January 1926, before his first paper on (non-relativistic) wave mechanics. How far did Schrödinger carry his relativistic considerations? What were their role in the genesis of wave mechanics? Were they prior to his treatment of the non-relativistic case?

There is, of course, the evidences from the published account in the "Quantisierung" series, such as reviewed in the preceding section. From this we definitely know that the relativistic treatment was known to Schrödinger before 27 January. But the published articles do not tell us whether the relativistic attempt was before or after the non-relativistic attempt.

A historical reconstruction of Schrödinger's route to wave mechanics has, therefore, to rely on unpublished material. And this appears to be a rather intricate historiographic problem: Partly due to lack of detailed prima facie sources, and partly to the fact that existing sources disagree on some essential points. For the first thing, Schrödinger has never himself accounted for how he was led to wave mechanics, except from what may be glimpsed from various casual remarks in letters and articles. Unlike most others of the leading quantum pioneers, he did never write a biography, nor any reminiscences of this crucial phase in modern physics. "Ich habe keinen solchen Respekt vor meiner Persönlichkeit, dass ich mich hinsetze und mühsam Vergangenes zusammenschreibe," Schrödinger once said with an overstated modesty.[154] Also the recent fashion in preserving historical sources by collecting statements from scientists involved in pioneering research, came a little too late to include any interviews with Schrödinger, who died in 1961 after some years of illness. The AHQP sources do not, unfortunately, cover any interviews with the founder of wave mechanics.[155]

In lack of autobiographical statements, the most important source to information about Schrödinger's route to wave mechanics has been the memoirs of Dirac. This scientist has on several occasions told his version about the genesis of wave mechanics.[156] The following is one example of Dirac's narrative:

> "Now there is one point that you might wonder about when you read of Schrödinger's work. Schrödinger developed his quantum mechanics from de Broglie's wave equation. De Broglie's wave equation was relativistic, and Schrödinger of course was profoundly influenced by the beauty of relativity, and you may wonder why it is that his work, where he introduces the wave equation, is nonrelativistic. There is a contradiction there.
>
> Schrödinger explained this matter to me many years later, I do not remember just when, around about 194o, when I had got to know him well. He said that he was working from the relativistic point of view inspired by de Broglie, and he was led to a relativistic wave equation, which was a generalization of de Broglie's equation, bringing in the electromagnetic potentials. When he got this relativistic equation, his first concern was to apply it to the hydrogen atom to see what results it would give. The calculation gave results that were not in agreement with observation.

> Schrödinger was extremely disappointed by that and thought that his wave equation was no good at all, and abandoned it. He gave it up for some months, then went back to it, and taking a second look at it, he noted that, if he used the equation with less accuracy in nonrelativistic approximation, the results that he got were in agreement with the experimental results, again with neglect of relativistic effects. So he was able to publish his wave equation in a nonrelativistic form, and in agreement with experiment.
>
> Of course, the reason why Schrödinger's original equation, the relativistic one, did not agree with experiment was because it did not take into account the spin of the electron. The spin of the electron was a very new idea at the time, and possibly Schrödinger had never even heard of it. And Schrödinger then did not have the necessary boldness to publish an equation which definitely gave results in disagreement with observation."[157]

Dirac's story is uncritically repeated in most historical studies on the subject.[158] Raman and Forman, however, have taken a more critical look at it, and merely regard it as an anecdote.[159] It may be useful to follow Raman and Forman and divide the message of the story in two parts: First, according to the story, Schrödinger worked out the relativistic problem before the publication of Q_1 and even before he tried to solve the non-relativistic equation; second, the disagreement as to the fine-structure caused Schrödinger to interrupt his original research programme for a couple of months. In one of the versions,[160] Dirac even claims that the relativistic attempt did not only delay wave mechanics for some months, but that the relativistic equation, first published by Klein in the spring 1926, was actually "discovered a year or two earlier by Schrödinger". However, while there are very good reasons to believe in the first part of Dirac's story, the latter part is not reliable. The creative phase of (relativistic) wave mechanics did not take place in the summer of 1925, and certainly not a year before, but in a short time-interval around the New Year 1925/26, Now, which evidences exist to justify or to correct Dirac's story?

(1) The American physicist D.M.Dennison, who worked with Schrödinger in Zürich in the autumn of 1926 and at later occasions, has recalled a meeting with Schrödinger from 1927. There, "he told me that his first attempt, in which he used relativistic mechanics, had not turned out well at all. He had the manuscript of it, but he never sent it in because it did not give the correct energy levels."[161]

(2) When Schrödinger was an old man, he reported about his relativistic attempt in a letter to Yourgraw and Mandelstam:

> "Sommerfeld's derivation of the fine-structure formula provides only fortuitously the result demanded by experiment. One may notice then from this particular example that the newer form of quantum theory (i.e., quantum mechanics) is by no means such an inevitable continuation of the older theory as is commonly supposed. Admittedly the Schrödinger theory, relativistically framed (without spin), gives a formal expression of the finestructure formula of Sommerfeld, but it is incorrect owing to the appearance of half-integers instead of integers. My paper in which this is shown has... never been published; it was withdrawn by me and replaced by the non-relativistic treatment... The computation [by the relativistic method] is far too little known. It shows in one respect how neccessary Dirac's improvement was, and on the other hand that it is wrong to assume that the older form of quantum theory is 'broadly' in accordance with the newer form."[162]

The information gained from this interesting letter seems to agree well with the accounts of Dirac and Dennison, though the question of when the relativistic study took place is still open. Also it may be worth to point out, that the ageing Schrödinger not only confirms that he prepared an early paper on relativistic wave mechanics; it is furthermore stated that he actually submitted the paper for publication. That is, Schrödinger sent the manuscript to Wien, co-editor of the *Annalen* (the other editor was Planck), and Schrödinger's favourite connection for publication (see note 178). This statement evidently disagrees with Dennison's statement that "he never sent it in." Anyhow, Schrödinger at some time prior to "Quantisierung" prepared a manuscript on relativistic wave mechanics. Unfortunately, this manuscript seems to have been lost.[163]

(3) Still another reminiscence is due to Erwin Fues who worked with Schrödinger in Zürich from November 1925 to December 1926. In an exchange of letters with Thomas Kuhn, Fues has accounted for his reminiscenses of the birth of wave mechanics.[164] Schrödinger's early relativistic attempt, Fues recalled, was before his arrival to Zürich:

> "Schrödingers erster, relativistischer Versuch zur Aufstellung einer Wellengleichung war schon abgeschlossen und ad acta gelagt, als ich hinkam (Nov.1925). Als wir das erste Gespräch über die Schrödingergleichung hatten, handelte es sich nach meiner Erinnerung nur um die unrelativistische. Deren Erfolg stand so sehr im Vordergrund dass ich das Versagen des ersten Versuchs lange Zeit gar nicht erfuhr (oder überhörte?)."[165]

If Fues' memory is to trust, the relativistic attempt should rather be dated to the summer of 1925, such as assumed by Gerber and others, and agreeing with Dirac's statement that Schrödinger abandoned the matter "for some months."

(4) There are, however, strong evidences that Schrödinger had *not* in his hands any wave equation for particles, whether relativistic or non-relativistic, prior to mid-November 1926. This is testified particularly by the letters to Einstein and Landé, such as quoted in §2. These letters show that Schrödinger did not apply de Broglie's ideas to problems of atomic structure until *c.* mid-November. The same thing may be inferred from a letter to Planck of 26 February 1926, where Schrödinger sketches his ideas of wave mechanics so far developed:

> "Darf ich Ihnen noch ganz kurz von einer Sache berichten, die mich *seit zwei Monaten* vollkommen gefangen nimmt und die - ich bin jetzt schon ganz fest überzeugt davon - eine ganz ausserordentliche Tragweite besitz."[166]

Additional evidence in support of the same thing may be obtained from the following passage in a letter to Wien:"... der Matrizenkalkül unerträglich war lange bevor ich an meine Theorie auch nur entfernt dachte...", Schrödinger wrote.[167] Since matrix mechanics developed in the summer of 1925, Schrödinger cannot have had his ideas about a wave mechanics at that time.

(5) Schrödinger's early occupation with a relativistic wave equation was also stressed in the letter to Lorentz of 6 June 1926, such as quoted in § 3. Years after the relativistic equation had been introduced by Klein, Gordon a.o., Schrödinger felt obliged to maintain his priority. When his close friend Hermann Weyl in the second edition of his *Gruppentheorie und Quantenmechanik* published the wave equation (6.5) under the name "de Broglie's equation", and also attributed the operator prescription (5.22) to de Broglie, Schrödinger protested:

> "Andernfalls aber ist es doch wirklich etwas störend, unter der Spitzmarke de Broglie beispielsweise die Operatorenzuordnung ($p_\ell \to \partial/\partial q_\ell$) zu lesen, die meines Wissens wirklich zum ersten Mal in meiner Note von 18.III.1926 mitgeteilt ist, und ebenso die skalar-relativistische Gleichung, die ich auf der ersten Seite meiner ersten Abhandlung (freilich nur mit worten) beschrieben und über deren Lösungen ich im §3, al 2 derselben Abhandlung eine Mitteilung gemacht habe. Ich habe nie dagegen protestiert, dass diese Gleichung jetzt ganz allgemein unter dem Namen Gordon läuft, denn das ist zur Unterscheidung sehr bequem. Unter dem Namen de Broglie sehe ich sie aber aus naheliegenden Gründen doch nicht sehr gern..."[168]

(6) Finally, the most detailed and reliable information about Schrödinger's early relativistic attempt may be gained from his voluminious research notebooks. These notebooks show conclusively that Schrödinger did indeed start his wave attack on atoms on a relativistic background and that it was only afterwards that he turned to a non-relativistic approximation, considered only to be a more manageable substitution for the real thing. Seven years later Schrödinger commented:

> "Les difficultés que nous avons rencontrées en tâchant de tenir compte du point de vue relativiste dans la mécanique quantique me semblent d'autant plus intéressantes qu'elles sont tout à fait *imprévues*. Vous savez que la mécanique nouvelle, sous la forme de mécanique *ondulatoire* sous laquelle elle est appliquée presque universellement aujourd'hui, doit son origine aux célèbres recherches de M.L.de Broglie, à son ingénieuse conception des ondes électroniques qui devaient accompagner le mouvement de l'électron. Les recerches de M.L.de Broglie s'appuyaient sur la théorie de la relativité restreinte; elles étaient pour ainsi dire imprégnées de relativité. Lorsqu'on les prit comme point de départ pour en tirer l'équation d'ondes et les problèmes de valeurs propres, on éprouva un peu de honte d'étre obligé de *supprimer* d'abord le point de vue relativiste et on espéra que ce ne serait qu'une situation provisoire et de courte durée, et qu'il ne serait pas trop difficile d'introduire la relativité à nouveau dans les équations. Mais au lieu de diminuer, il semble bien que cette difficulté a crû d'une année à l'autre jusqu'à prendre aujourd'hui des proportions effrayantes."169

The relevant parts of Schrödinger's research notebooks will be wubjects to a closer examination in the following section.

§ 8. SCHRÖDINGER AND THE RELATIVISTIC KEPLER PROBLEM.

During most of his career, Schrödinger recorded the progress of his scientific research by means of a system of notebooks, most of which have been microfilmed by AHQP.[170] Unfortunately, most of these notebooks are undated, so in the assumed datings there cannot avoid to be a certain arbitrariness. The datings given by AHQP cannot be much wrong, however; they are in good agreement with the analysis of the present study.

The notebooks, of particular relevance to the genesis and first development of Schrödinger's wave mechanics, are the following:

N_1: "H Atom, Eigenschwingungen", 3 pp. Late 1925 or early January 1926.

N_2: "Eigenwertproblem des Atoms, I", 72 pp. Late 1925 or January 1926.

N_3: "Eigenwertproblem des Atoms, II (Allgemeine Theorie)", 48 pp. c. February 1926.

N_4: "Starkeffekt fortgesetzt," 16 pp. c. February 1926.

N_5: "Eigenwertproblem des Atoms, III", 48 pp. c. March 1926.

N_6: "Dirac," 24 pp. May or June 1926.

Of these sources, particularly N_1, N_2 and N_6 are valuable as to the genesis of wave mechanics. While N_1 and N_2 are a collection of rough notes and unfinished calculations, which have only a remote resemblance with the content of the first published communication, N_3, N_4 and N_5 appear in a much less tentative form; evidently they are rough drafts to Q_2 and Q_3 whose contents they largely follow. Comparison of N_1 and N_2 shows that N_1 is written before N_2. The N_1 notes are, then, of particular interest, since they are the very first evidence for Schrödinger's occu-

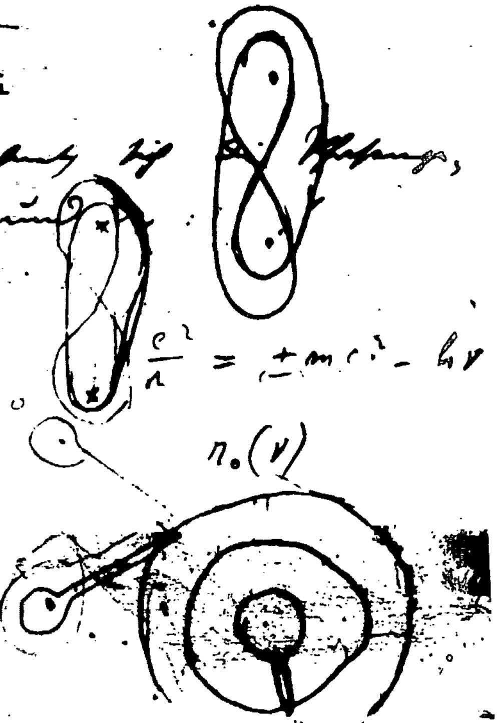
1) [illegible] Elektron, Dispersion der Phasenwelle,

$$\nu = \frac{mc^2}{h\sqrt{1-\beta^2}} \qquad u = \frac{c}{\beta} = \frac{c^2}{v} = \frac{\frac{mc^2}{\sqrt{1-\beta^2}}}{\frac{mv}{\sqrt{1-\beta^2}}} = \frac{1\ \text{Energie}}{1\ \text{Impuls}}$$

2.) Vorläufige Übertragung auf das Elektron im Kernfeld.

$$h\nu = \frac{mc^2}{\sqrt{1-\beta^2}} - \frac{e^2}{r} \qquad u = \frac{h\nu}{\frac{mv}{\sqrt{1-\beta^2}}}$$

Durch Elimination von v (oder β) bekommt man die Phasengeschwindigkeit u als Funktion von ν und r:



$$u = c\,\frac{\frac{h\nu}{mc^2}}{\sqrt{\left(\frac{h\nu}{mc^2}+\frac{e^2}{mc^2 r}\right)^2-1}}$$

$$\frac{e^2}{r} = \pm mc^2 - h\nu$$

$r_0(\nu)$

$$e^{2\pi i\nu t}$$

$$\Delta\psi = -\frac{4\pi^2\nu^2}{u^2}\psi$$

$$= -\frac{4\pi^2}{h^2}m^2c^2\left(\left(\frac{h\nu}{mc^2}+\frac{e^2}{mc^2 r}\right)^2-1\right)\psi$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{\partial}{\partial\vartheta} \quad \frac{\partial}{\partial\varphi} = -Q\psi$$

$$-n(n+1)\psi$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \left(Q - \frac{n(n+1)}{r^2}\right)\psi = 0$$

$$\frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r} + \qquad \psi = r^{-\frac{1}{2}}\chi$$

$$\frac{\partial^2\chi}{\partial r^2} + \frac{1}{r}\frac{\partial\chi}{\partial r} + \underbrace{\left(Q - \frac{(n+\frac{1}{2})^2}{r^2}\right)}\chi = 0 \qquad (2n+1)^n$$

$$\pm i\sqrt{a}$$

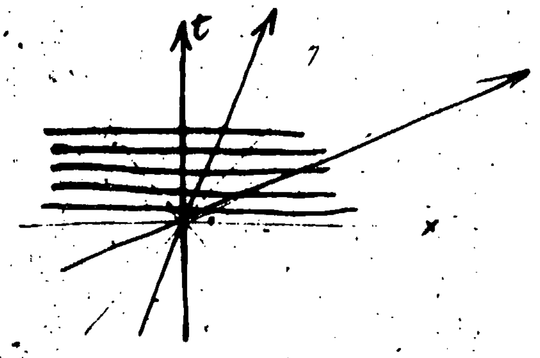
$$\oint\sqrt{Q-\frac{(n+\frac{1}{2})^2}{r^2}}\,dr = 2\pi. \qquad \underline{\alpha^2 = c}$$

$$\frac{d^2J}{dr^2} + \frac{1}{r}\frac{dJ}{dr} + \left(-a + \frac{2b}{r} - \frac{c}{r^2}\right)J = 0.$$

$$J = r^\alpha u \qquad r^\alpha u'' + r^{\alpha-1}u'(2\alpha+1) + r^{\alpha-2}u\left(\cancel{\alpha^2 - c} - ar^2 + 2br\right) = 0$$

$\nu = \frac{mc^2}{h}$ $\qquad \nu = \frac{mc^2}{h\sqrt{1-\beta^2}}$ $\qquad u = \frac{c}{\beta} = \frac{c^2}{v}$

$u(\nu)$



$$u = \frac{\frac{mc^2}{\sqrt{1-\beta^2}}}{\frac{mv}{\sqrt{1-\beta^2}}} = \frac{\frac{mc^2}{\sqrt{1-\beta^2}} - \frac{e^2}{r}}{\frac{mv}{\sqrt{1-\beta^2}}} = \frac{h\nu}{}$$

$\frac{h\nu}{mc^2} = \frac{\nu}{\nu_0}$ $\qquad u = c\,\frac{\frac{\nu}{\nu_0}}{\sqrt{\left(\frac{\nu}{\nu_0}+\frac{a}{r}\right)^2 - 1}}$ $\qquad \sqrt{\ } = 0 = \sqrt{\left(\frac{a}{r}+\frac{\nu}{\nu_0}+1\right)\left(\frac{a}{r}+\frac{\nu}{\nu_0}-\right)}$

$\frac{e^2}{mc^2} = a$ $\qquad \frac{\nu}{\nu_0} + \frac{a}{r} = \pm 1$

$\frac{a}{r} = -\frac{\nu}{\nu_0} \pm 1$

$\frac{4\pi^2\nu_0^2}{c^2} = k^2$ $\qquad \Delta\psi = -\frac{4\pi^2\nu_0^2}{c^2}\left(\left(\frac{\nu}{\nu_0}+\frac{a}{r}\right)^2 - 1\right)\psi$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \left[k^2\left(\left(\frac{\nu}{\nu_0}+\frac{a}{r}\right)^2 - 1\right) - \frac{n(n+1)}{r^2}\right]\psi = 0$$

$-A = k^2\frac{\nu^2}{\nu_0^2} - k^2 = \frac{4\pi^2\nu^2}{c^2} - \frac{4\pi^2\nu_0^2}{c^2} = -\frac{4\pi^2}{c^2}(\nu_0^2 - \nu^2)$

$B = \frac{k^2\nu}{\nu_0}a = \frac{4\pi^2}{c^2}\nu\nu_0 a$

$-C = k^2a^2 - n(n+1)$; $\quad C = n(n+1) - k^2a^2$; $\quad C + \frac{1}{4} = (n+\frac{1}{2})^2 - k^2a^2$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \left[-A + \frac{2B}{r} - \frac{C}{r^2}\right]\psi = 0$$

$\psi = r^\alpha u$ $\qquad r^\alpha u'' + 2(\alpha+1)r^{\alpha-1}u' + r^{\alpha-2}u\left(2\alpha + \alpha(\alpha-1) - Ar^2 + 2Br - C\right) = 0$

$\psi' = \alpha r^{\alpha-1}u + r^\alpha u' \quad \Big| \ \frac{2}{r}$ $\qquad \alpha(\alpha+1) = C$

$\alpha = -\frac{1}{2} \pm \sqrt{\frac{1}{4} + C}$

$\psi'' = \alpha(\alpha-1)r^{\alpha-2}u + 2\alpha r^{\alpha-1}u' + r^\alpha u''$

$2(\alpha+1) = 1 \pm 2\sqrt{C + \frac{1}{4}}$

$r u'' + 2(\alpha+1)u' + (-Ar + 2B)u = 0$ $\qquad$ α kann zwei Werte haben!

$\delta_0 = 0 \quad \delta_1 = 2(\alpha+1) \qquad \varepsilon_0 = -A \qquad \varepsilon_1 = 2B$

$q = z^2 + 0\cdot z + (-A) = 0 \qquad \left.\begin{matrix} c_1 \\ c_2 \end{matrix}\right\} = \pm\sqrt{A}$ in beiden Fällen.

$\alpha_1 = \frac{\varepsilon_1 + \delta_1 c_1}{c_1 - c_2} = \frac{2B + 2(\alpha+1)\sqrt{A}}{2\sqrt{A}}$ $\qquad \alpha_2 = \frac{\varepsilon_1 + \delta_1 c_2}{c_2 - c_1} = \frac{2B - 2(\alpha+1)\sqrt{A}}{-2\sqrt{A}}$

$c_1 - c_2 = 2\sqrt{A}$

$c_1 = +\sqrt{A} \qquad c_2 = -\sqrt{A}$

1) $\alpha = -\frac{1}{2} + \sqrt{C + \frac{1}{4}}$

$$a_1 = \frac{B}{\sqrt{A}} + \sqrt{C + \tfrac{1}{4}} + \frac{1}{2}$$

$$a_2 = -\frac{B}{\sqrt{A}} + \sqrt{C + \tfrac{1}{4}} + \frac{1}{2}$$

2) $\alpha = -\frac{1}{2} - \sqrt{C + \frac{1}{4}}$

$$a_1 = \frac{B}{\sqrt{A}} - \sqrt{C + \tfrac{1}{4}} + \frac{1}{2}$$

$$a_2 = -\frac{B}{\sqrt{A}} - \sqrt{C + \tfrac{1}{4}} + \frac{1}{2}$$

[illegible] A, B, C [illegible] $\frac{4\pi^2}{h^2}$.

~~[illegible]~~

~~[illegible] a_1, a_2 [illegible]~~ !!!!!!!!!!!!!!!!

[illegible] ! [illegible] ?

[illegible]:

$$\frac{1}{u^2}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2u^2\frac{\partial\psi}{\partial r} + \frac{u^2}{r^2}\left(\frac{\partial}{\partial\theta} \cdots -\{n(n+1)\}\right)\right) = -\frac{4\pi\nu^2}{u^2}\psi \qquad u^{\alpha-1}\frac{\partial u}{\partial r} \quad u^{-\alpha}$$

[illegible]:

$$\frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r} - \frac{2}{u}\frac{\partial u}{\partial r}\frac{\partial\psi}{\partial r} + \left[-A + \frac{2B}{r} - \frac{C}{r^2}\right]\psi = 0$$

$$\frac{\partial \lg u}{\partial r} = +\frac{1}{4}\left(\frac{\nu}{\nu_0} + \frac{a}{r}\right)\frac{a}{r^2}$$

The original content of Erwin Schrödinger's first notes on wave mechanics (N_1), in which the famous Schrödinger eigenvalue equation appears for the first time and is unsuccessfully applied to the hydrogen atom.

pation with wave mechanics. Apart from the notebooks, mentioned above, Schrödinger wrote five notebooks on "Relativistische Quantenmechanik," which are not contained in the AHQP archive. It turns out, however, that this material does not deal with the early period, here considered.[171]

In N_1, Schrödinger made a straightforward application of de Broglie's formulae under the heading "Vermutliche Übertragung auf das Elektron im Raumfeld." Closely following de Broglie, the phase velocity of the wave associated with the bound electron is expressed as a function of its frequency and the radius of the classical orbit. From

$$V = \frac{E}{p} = \frac{h\nu\sqrt{1-\beta^2}}{m_0\beta c} \quad \text{and} \quad h\nu = \frac{m_0c^2}{\sqrt{1-\beta^2}} - \frac{e^2}{r}$$

(which formulae also appeared in de Broglie's thesis, cf. (1.13) and (1.14)) the signal velocity $\beta=v/c$ is eliminated so as to get

$$V = c\,\frac{\dfrac{h\nu}{m_0c^2}}{\sqrt{\left(\dfrac{h\nu}{m_0c^2} + \dfrac{e^2}{m_0c^2r}\right)^2 - 1}}$$

To obtain the wave equation, this expression is inserted in the general space form of the amplitude equation

$$\Delta\psi + \frac{4\pi^2\nu^2}{V^2}\,\psi = 0 \tag{8.1}$$

with the result

$$\Delta\psi + \frac{4\pi^2}{h^2}\,m_0^2c^4\left[\left(\frac{h\nu}{m_0c^2} + \frac{e^2}{m_0c^2r}\right)^2 - 1\right]\psi = 0 \tag{8.2}$$

This is the equation such as written by Schrödinger in N_1. If we put $E=h\nu$, the equation is reckoned to be the relativistic Schrödinger equation, the so-called Klein-Gordon equation.

It should be noticed that this original way of deriving the wave equation is very different from the methods which were published in Q_1 and Q_2. It is much simpler, and it rests crucially on de Broglie's theory. Since this theory was relativistic, the outcome of Schrödinger's first attempt naturally was a relativistic wave equation. In the few sheets of the N_1 notes, there is no trace of a non-relativistic treatment. (8.2) is no doubt the first appearance of the famous (relativistic) Schrödinger equation. It was probably written in the latter part of December 1925.

Schrödinger naturally tried to solve the equation in the fair hope that it would yield for the energy Sommerfeld's fine-structure formula. However, the wave mechanical eigenvalue equation involves mathematics which was far from standard at the time. It caused Schrödinger great mathematical difficulties, such as is reflected in his letter to Wien of 27 December (see §2). "Wenn ich nur mehr Mathematik könnte!" As we shall see, Schrödinger was not able to find a solution, neither in N_1 nor in the slightly later N_2. But probably in the second week of 1926 Schrödinger surmounted the troubles and found the energy spectrum of his relativistic hydrogen atom according to wave mechanics. In the treatment of the energy equation, Schrödinger was assisted by the mathematical skill of Hermann Weyl who at the time was Schrödinger's colleague as a professor at the University of Zürich.[172] During his attempts to solve the differential equation which determines the energy spectrum, Schrödinger relied on an older textbook by Ludwig Schlesinger, professor at the University of Giessen.[173] This shows that even if the mathematics of the Schrödinger equation was unfamiliar to most physicists, it was not at all new to the mathematicians. In fact, the so-called Laplace equation which was the mathematical core of Schrödinger's theory for the hydrogen atom, was first considered in 1812 by Laplace. The general theory for equations of this kind was worked out by H.Poincaré in 1885 and further developed by J.Horn in 1897.[174] It was this theory, in Schlesinger's presentation, that was applied by Schrödinger in Q_1. Most likely, Schrödinger has also benefitted from the detailed exposition of eigenvalue problems in Hilbert and Courant's newly published textbook on mathematical physics.[175] It is remarkable, however, that Schrödinger does nowhere in Q_1 refer to Hilbert and Courant, while there are numerous references (sixteen, in fact) to this book in his other papers on wave mechanics.

In Q_1 Schrödinger gave a detailed treatment of the (non-relativistic) eigenvalue equation (6.5), and demonstrated that its radial part results in Bohr's formula (3.1). The radial part of the wave equation was, as usual, obtained by substituting $\psi(r, \varphi, \theta)$ with $Y(\varphi, \theta)\cdot\chi(r)$ in (5.12). Then, by insertion

$$\frac{d^2\chi}{dr^2} + \frac{2}{r}\frac{d\chi}{dr} + \left(A + \frac{2B}{r} + \frac{C}{r^2}\right)\chi = 0 \tag{8.3}$$

where

$$A = \frac{8\pi^2 m}{h^2}(E-mc^2), \qquad B = \frac{4\pi^2 me^2}{h^2}, \qquad C = -n(n+1) \tag{8.4}$$

(E denotes, here and elsewhere in this section, the relativistic energy). From the relativistic equation, exactly the same form comes out, only that the coefficients have now different values:

$$\left.\begin{aligned} A &= \frac{4\pi^2}{c^2h^2}(E^2-m_0^2c^4) \\ B &= \frac{4\pi^2e^2}{c^2h^2}E \\ C &= \frac{4\pi^2e^2}{c^2h^2} - n(n+1), \qquad n = 0,1,2,\ldots \end{aligned}\right\} \tag{8.5}$$

In (8.4) as in (8.5), the 'quantum number' n appears as a purely mathematical quantity, viz, as the order of the spherical harmonic $Y(\varphi, \theta)$.

In both of Schrödinger's early notebooks, N_1 and N_2, he starts out from (8.3) (using a slightly different notation) and he applies a similar mathematical technique as the one only successfully completed in Q_1. In there, Schrödinger analyzed the behaviour of $\chi(r)$ at the singularities $r = 0$ and $r = \infty$ and showed that at $r = 0$ the solution may be represented by the power series

$$\chi = r^n \sum_{\nu=o}^{\infty} a_\nu r^\nu$$

He then proceeded with the substitution

$$\chi = r^\alpha U$$

which transforms (8.3) into

$$\frac{d^2U}{dr^2} + \frac{2(\alpha+1)}{r}\frac{dU}{dr} + (A + \frac{2B}{r}) = o \qquad (8.6)$$

In N_1 the same procedure is followed. However, from here the difficulties begin, if I am not mistaken. In the non-relativistic case in Q_1, the so-called indicial or characteristic equation ("determinierende Fundamentalgleichung") reveals that α may attain the values n or $-(n+1)$; but in Q_1 Schrödinger argued that both of these values lead to the same solution, and he therefore considered only the case $\alpha = n$. In the relativistic case, such as pictured in N_1, the corresponding α values turn out to be

$$\alpha = -\frac{1}{2} \pm \sqrt{C + \frac{1}{4}} \qquad (8.7)$$

(which, in the non-relativistic limit, give n or $-(n+1)$). With (8.6), Schrödinger, in the calculations given in N_1 and N_2, apparently proceeds in a similar way as in Q_1. That is, (8.6) is noticed to be a so-called Laplace equation, whose general form, copying Schlesinger's textbook, is written as

$$\frac{d^2U}{dr^2} + (\delta_0 + \frac{\delta_1}{r}) \frac{dU}{dr} + (\varepsilon_0 + \frac{\varepsilon_1}{r})U = 0 \qquad (8.8)$$

where now

$$\delta_0 = 0, \qquad \delta_1 = 2(\alpha+1), \qquad \varepsilon_0 = A, \qquad \varepsilon_1 = 2B$$

The standard solution of (8.8), again taken over from Schlesinger' is a curve integral in the complex plane, of the general form

$$U = \int_L e^{zr}(z - c_1)^{\alpha_1 - 1} (z - c_2)^{\alpha_2 - 1} dz$$

where c_1 and c_2 are the roots of

$$z^2 + \delta_0 z + \varepsilon_0 = 0$$

and where

$$\alpha_1 = \frac{\varepsilon_1 + \delta_1 c_1}{c_1 - c_2}, \qquad \alpha_2 = \frac{\varepsilon_1 + \delta_1 c_2}{c_2 - c_1}$$

For Schrödinger's relativistic case, this gives

$$c_1 = \sqrt{-A}, \qquad c_2 = -\sqrt{-A}$$

$$\alpha_1 = \frac{B}{\sqrt{-A}} + \alpha + 1, \qquad \alpha_2 = -\frac{B}{\sqrt{-A}} + \alpha + 1 \qquad (8.9)$$

These are also the results of Q_1 (where $\alpha = n$). The crucial step concerns the values of α_1, α_2. In Q_1 Schrödinger concluded after a lengthy analysis, that for bound states ($E < 0$) there are only solutions to the problem if α_1 and α_2 are both integers. This means that $B/\sqrt{-A}$ must also be an integer, viz.

$$\frac{B}{\sqrt{-A}} = \ell, \quad \ell = 1,2,3,\ldots \tag{8.10}$$

This formula is actually Bohr's expression for the energy levels of the hydrogen atom, such as may be seen if the values for A and B are inserted from (8.4). Also in N_1 the formulae (8.9) were obtained, but Schrödinger was at this occasion not able to proceed further. He ends up with four α_1, α_2 values, corresponding to the two signs in (8.7):

$$\left.\begin{aligned} \alpha_1 &= \frac{B}{\sqrt{-A}} \pm \sqrt{C + \frac{1}{4}} + \frac{1}{2} \\ \alpha_2 &= \frac{B}{\sqrt{-A}} \pm \sqrt{C + \frac{1}{4}} + \frac{1}{2} \end{aligned}\right\} \tag{8.11}$$

The meaning of these expressions is reckoned if the values of A, B and C are inserted. If Sommerfeld's fine-structure constant, here called f (to avoid confusion with the other α's), is introduced ($f = e^2 2\pi h^{-1} c^{-1}$), we get:

$$\alpha_{1,2} = \pm \frac{f}{\sqrt{\left(\frac{m_o c^2}{E}\right)^2 - 1}} \pm \sqrt{(n + \tfrac{1}{2})^2 - f^2} + \frac{1}{2}$$

Apparently Schrödinger was uncertain about how to decide about the permitted values of α_1 and α_2. In N_1 he comments on the expression (8.11) in the following words:

> "Es muss nun so sein, dass einer von diesen beiden Exponenten ganz sein muss: Das ist die endliche [?] Quantenbedingung. Denn unsere A,B,C tragen gegenüber der Sommerfeldschen noch den Faktor
> $$\frac{4\pi^2}{h^2}$$
> NB: ~~$\alpha_1+\alpha_2$ ist ganzzahlig!~~ [this sentence is crossed out by Schrödinger].
> ~~Also werden dann α_1,α_2 beide ganzzahlig!!!!!!!!!!!!!!~~ [also this sentence is crossed out].
> Wenn man nun aber statt der Dichte die Elektrizität variabel ansetzt! Was dann?"

Here follows a few rough calculations and the note stops abruptly. In N_2 the problem is taken up again under the heading "Zur Ausarbeitung des vorläufig Erreichen zur Lösung der Laplaceschen Gleichung". But neither at this stage is Schrödinger able to reach a conclusion as to the evaluation of (8.11).

Schrödinger's original solution of the relativistic Kepler problem is not included in his left notebooks. It is only from a later notebook, entitled "Dirac" (N_6), that we can follow the solution in details. It contains some comments on Dirac's quantum mechanical theory, but most of it is occupied with Schrödinger's own theory. The relativistic Kepler problem is probably recalculated in connection with the chapter on relativistic wave mechanics which appeared in Q_4 (cf. § 6). Schrödinger's method to solve eq.(8.6) in N_6 is somewhat different from the non-relativistic method of Q_1, and likely it is also slightly different from Schrödinger's original treatment of January 1926. In N_6 Schrödinger takes, for instance, advantage of the properties of Laguerre polynomials in expressing the radial eigen-solutions; in January, Schrödinger did not fully recognise the relevance of Laguerre polynomials to his radial equation.[176] Incidentally, Schrödinger's treatment of the relativistic Kepler problem in N_6 is essentially the same which may be found in later textbooks.[177]

The main points are: In (8.7) the minus sign is discarded, so that

$$\alpha = -\frac{1}{2} + \sqrt{C + 1/4} \quad = \quad \sqrt{(n + \frac{1}{2})^2 - f^2} - \frac{1}{2}$$

Then eq.(8.6) is rewritten with the substitution

$$U = e^{-x/2} \cdot L_\nu(x)$$

where $x = 2r\sqrt{-A}$. The radial equation then takes the form

$$\frac{d^2 L}{dx^2} + \left[\frac{2(\alpha + 1)}{x} - 1\right] \cdot \frac{dL}{dx} + \left[\frac{B}{\sqrt{-A}} - \alpha - 1\right] \cdot \frac{1}{x} \cdot L = o \qquad (8.12)$$

If now L is expressed as a series, $\sum_0^\infty a_\nu x^\nu$, a recurrence formula for a_ν comes out from (8.12), viz.

$$[(\nu+1)(\nu+2\alpha+2)]a_{\nu+1} \quad = (\nu - \frac{B}{\sqrt{-A}} + \alpha + 1)a_\nu$$

For regular solutions the series must cease, say, at $\nu = n'$, so that

$$n' - \frac{B}{\sqrt{-A}} + \alpha + 1 = o$$

where n' is then an integer. Introducing the values for B, A and α, we have

$$\frac{f}{\sqrt{\left(\frac{m_o c^2}{E}\right)^2 - 1}} \quad = n' + \sqrt{(n + \frac{1}{2})^2 - f^2} + \frac{1}{2}$$

Finally, this equation gives after some manipulation:

$$E = \frac{m_0 c^2}{\sqrt{1 + \dfrac{f^2}{\left[(n' + \frac{1}{2}) + \sqrt{(n+\frac{1}{2})^2 - f^2}\right]^2}}} \qquad (8.13)$$

This is Schrödinger's result, such as stated in N_6, and such as it must have been found some time in January 1926.

When Schrödinger found (8.13) to be the result of his laborious calculations, it must have been with mixed feelings: The formula has the general structure of Sommerfeld's fine-structure formula, but the quantum numbers (radial and azimuthal) are wrong, half-integers instead of integers. So near to, and so far away! The discrepancy is serious, since the excellent agreement between Sommerfeld's formula and the spectroscopic experience is now destroyed. This is seen from the second-order approximation of (8.13), which is

$$E = -\frac{Rh}{n^2}\left[1 + \frac{f^2}{m^2}\left(\frac{m}{n+\frac{1}{2}} - \frac{3}{4}\right)\right]$$

with

$$m = (n' + \tfrac{1}{2}) + (n + \tfrac{1}{2}) = n' + n + 1$$

Compare with the approximate Sommerfeld formula (3.3). While the H_α doublet has a separation in frequency of $\frac{Rf^2}{16}$ according to Sommerfeld's theory (cf. § 3), the separation now becomes

$$\Delta\nu = \frac{Rf^2}{16}(4 - 4/3) = \frac{8}{3}\frac{Rf^2}{16}$$

which is far larger than permitted by measurements. So although Schrödinger succeeded in deriving a promising formula, it was definitely a false one.

§9. THE TURN TO NON-RELATIVISTIC WAVE MECHANICS

When Schrödinger found the energy values of the relativistic hydrogen atom according to his modification of de Broglie's ideas, the result must have been a serious disappointment because of the wrong quantum numbers, such as stated by Dirac. But Dirac's further account, that Schrödinger "thought that his wave equation was no good at all, and abandoned it," does not agree with what happened in January 1926.

Rather, Schrödinger may have decided to publish the calculations despite of their disagreement with experience, and he may have worked out a paper on the relativistic wave equation and its application to the hydrogen atom. This suggestion is justified by the evidences listed in §7. Schrödinger probably sent the manuscript to Wien for publication in the *Annalen*[178], although hesitatingly and in a mood of despair: on the one hand, Schrödinger had to admit that his theory failed in the sense that it did not reproduce the fine-structure correctly. On the other hand, Schrödinger did not therefore dismiss his wave equation as being "no good at all". And he was quite justified in keeping some confidence in the original, relativistic equation: the resemblance of his results with the exact Sommerfeld formula was too striking to be the result of an entirely wrong approach. Furthermore, Schrödinger's result was not so bad at all: it reproduced the general features of the fine-structure and it also gave the correct Balmer terms in the non-relativistic limit (eq. (8.13) reduces to Bohr's formula if $f^2 \to 0$). This was no small achievement, and particularly so since matrix mechanics had not yet solved the crucial hydrogen problem. As we saw in §4, the first matrix mechanical treatments of the hydrogen atom were submitted for publication only a couple of weeks after Schrödinger had obtained his result. For Pauli's theory, it had been accomplished already in November 1925. However, Schrödinger has probably not known about these attempts prior to their publication, and has thought that his wave mechanical analysis furnished the first new derivation of Bohr's formula for the hydrogen spectrum.

That Schrödinger should have seriously considered to abandon the whole matter because of the wrong fine-structure formula, seems completely unlikely.[179] So we may assume, following Schrödinger's own reminiscense (cf. the letter to Yourgraw and Mandelstam, §7), that he submitted the relativistic manuscript for publication in order to proceed with other aspects of his ambitious programme and to get responses from other physicists. Schrödinger may have paused for a few days, which would indeed be natural after his *tour de force*, still worrying about the lack of complete agreement in his theory for the hydrogen atom. He has then decided to sacrifice the relativistic ambitions for experimental agreement and has withdrawn his original manuscript. The revision of the manuscript into the form contained in Q_1 cannot have caused great problems to Schrödinger; probably it has only taken a few days. Since the mathematical analysis in the non-relativistic case follows the relativistic case very closely, it requires only minor modifications to present a coherent, non-relativistic theory.

In fact, this was not the first time that Schrödinger considered the non-relativistic approximation. On the first page of N_2, definitely written before he had solved the hydrogen case, Schrödinger thus considers the hydrogen atom "Ohne Relativistik (erste Näherung)". He starts with the approximation

$$E = h\nu = m_o c^2 + \tfrac{1}{2}mv^2 - {}^{e^2}/r$$

and, following the same de Broglie inspired procedure which first led to the relativistic equation (§8), he writes the wave equation as

$$\Delta\psi + \frac{8\pi^2 m_o}{h^2}(E - m_o c^2 + \frac{e^2}{r})\psi = 0$$

This is the usual Schrödinger equation, and probably the very first time it is written. In N_2 the radial part of this equation is examined with the same methods as applied to the relativistic equation in N_1, but with no better luck. Symptomatically for Schrödinger's early, relativistic programme, he then returns to the relativistic equation. From the content of the notebooks it appears that Schrödinger did, in large measure, consider the non-relativistic case only in the hope that it would yield a mathematically more manageable problem. Realizing that this is not so, Schrödinger temporarily gave it up.

Schrödinger's final presentation of his wave mechanics in a non-relativistic form then seems to be rooted in tactical considerations rather than expressing any change in Schrödinger's view on the nature of wave mechanics. Publishing a non-relativistic theory, the wave mechanical programme *appears* experimentally agreeable[180], fairly coherent and on the whole convincing to experimentalists as well as to theorists. There can be no doubt that Schrödinger, also after the publication of Q_1, considered wave mechanics to be completely satisfactory only if including relativity. This is manifest, not only from Schrödinger's published papers (see § 6) but also from his notebooks. In there, the relativistic attempts predominate over the non-relativistic ones. Not least in connection with the Zeeman effect, there are many unfinished attempts to treat it relativistically.

In N_4, written c. march 1926, Schrödinger tries to include relativistic effects in the hydrogen atom as perturbations ("Relativistik, als Störung aufgefasst"). Including the first-order relativistic correction, the energy is written as

$$E = m_0 c^2 (\tfrac{1}{2}\beta^2 + \tfrac{3}{8}\beta^4) - e^2/r$$

Schrödinger then formulates, using a variational procedure similar to that of Q_1, the wave equation as

$$\Delta\psi + \frac{2m_0}{K^2}\left[E - \frac{3E^2}{m_0 c^2} + \frac{e^2}{r}\left(1 - \frac{6E}{m_0 c^2}\right) - \frac{3e^4}{m_0 c^2 r^2}\right]\psi = o$$

where $K = {}^{h}/2\pi$. However, the attempt to solve this equation is fruitless.

One may wonder why Schrödinger derived his eigenvalue equation in Q_1 by the non-intuitive variational procedure (cf. § 5), instead of using de Broglie's formulae together with the spatial wave equation. The latter procedure was, as we have seen, presumably Schrödinger's original way to the relativistic wave equation. It may equally well be applied to a non-relativistic approximation, in which case 'de Broglie's formulae' take the forms

$$V = \frac{h\nu}{mv} \quad \text{and} \quad h\nu = \tfrac{1}{2}mv^2 - e^2/r$$

If these formulae are combined and $V=V(\nu)$ is inserted in the wave equation, the usual Schrödinger equation easily comes out.

When Schrödinger did not follow this simple method in his publications, it may have several reasons. For one thing, the method is not, being based on non-relativistic approximations, conceptually justified in de Broglie's thoroughly relativistic theory. For another thing, Schrödinger may have wanted to present his opening address on wave mechanics in a manner which did not connect it too closely to de Broglie's ideas; to the extent that these ideas were known to physicists outside Paris, they were still regarded as unrealistic and speculative.

§ 10. THE WAVE EQUATION AND GENERAL RELATIVITY: KLEIN'S APPROACH

To this and the following section, we shall briefly survey how the original - i.e. the relativistic - Schrödinger equation was derived and treated by quantum physicists in 1926. I have discussed the further fate of this equation, and how it was replaced by Dirac's linear equation in early 1928, in another study.[181] The relativistic wave equation was in 1926 derived and applied by some twenty authors, of whom some found it independently of Schrödinger. It was indeed a proper choice of name when Pauli called it 'the equation with the many fathers'.[182] In the following, we shall adopt the now standard usage of the second order relativistic equations (6.4) and (6.5), and call them the Klein-Gordon equations. Although in the period considered various other names were also in use.

The KG equation is a simple combination of wave mechanics and special relativity. Hitherto we have spoken about relativity as synonymous with the special theory. However, the first published account of the KG equation had its origin in considerations on general relativity, and the attempts to incorporate quantum mechanics in general relativity constituted a vigorous trend in the late twenties. Actually, the publications concerned with this hybrid field outnumbered the publications on special relativity quantum mechanics. In the following I shall deal mainly with this trend in connection with the theory of Oskar Klein, who was the first one to publish a relativistic wave equation.

Oskar Klein[183] was one of Bohr's first assistants in Copenhagen where he very soon showed remarkable talents in theoretical physics.[184] In particular, he made valuable contributions to the teasing problem of the energy perturbations in atoms when placed in crossed electric and magnetic fields; this problem turned out to be an unsurmountable obstacle to the old quantum theory, and Klein's work thus added another evidence to the general crisis of the Bohr-Sommerfeld theory (Klein's problem was first solved by Pauli, in his treatment of the hydrogen atom according to quantum mechanics (§ 4)). Apart from his work in the old quantum theory and related areas, Klein had from 1921 onwards also speculated about quantum problems in a completely different and original way, which was substantially like the one which guided de Broglie. Independently Klein reached, in private, to an understanding of some deep-rooted connection between particles, waves and quanta. As early as in 1922 he had become convinced that particles should somehow be related to self-interfering waves, and Klein imagined this relation to be formally connected to Hamilton's analogy between geometrical optics and particle mechanics.

Klein's early speculations about a wave interpretation of quantum theory departed from an idea, that the quantum conditions might in some way be due to interference of waves, an idea suggested by the appearance of whole numbers in both fields. Also, Klein soon began to think of quantization of stationary states as eigen-solutions to vibrations. These vague ideas he gradually connected with the Hamilton-Jacobi equation, regarded as a wave-front equation. In his search for a proper wave equation, Klein unfortunately complicated things by considering equations with non-linear terms, not realizing the necessity for a superposition principle. Furthermore, from 1924 Klein was led into a whirlwind of speculations, since he tried to combine his quantum ideas with studies on the formal similarities between, and possible unification of, Maxwell's electromagnetic equations and Einstein's gravitational field theory. Klein then got engaged in a most ambitious attempt to incorporate electromagnetism, quantum theory and general relativity in one grand synthesis. In this way Klein was led to a five-dimensional extension of relativity, in which framework he tried to express his wave view of quantum theory. At the time, 1924-25, when Klein worked out his theory of a five-dimensional unified theory, he was unaware that Kaluza had already published a five-dimensional theory of relativity. It was only in the spring of 1926 that he became aware, through Pauli, of Kaluza's work.

No doubt this comprehensive programme - which Klein, furthermore, wanted to work out with mathematical rigour - was too ambitious. Klein's otherwise so promising ideas, which could possibly even have led him to a complete wave mechanics prior to Schrödinger, were probably destroyed by this synthetical approach.[185] As Dirac later told Klein, his main trouble was that he tried to solve too many problems at the same time.[186] Apart from the almost impossible job Klein had devoted himself to, he was also handicapped because of lack of scientific response and cooperation. The shy Klein seems not to have discussed his vague and admittedly speculative ideas with his colleagues in Copenhagen or elsewhere.[187] And in most of 1923-25 Klein was a research assistant at the University of Michigan, at that time a rather isolated and less developed site as regards theoretical physics.

When Klein, in the spring of 1925, returned to Copenhagen, he eventually gave up his non-linear approach and began to consider the simple, linear wave equation. Latest in the summer of 1925 Klein had a kind of generalized wave equation which probably has contained Schrödinger's later equations as special cases.[188] While staying in USA, Klein did not know about de Broglie's theory, but in the summer of 1925 Bohr gave him a copy of de Broglie's thesis. He ran through it, but did not, at that time, recognize its profoundity and its relevance to his own speculations. Klein continued, interrupted by a long period of illness which made him inactive during the rapid development of quantum physics in the fall of 1925, his own attempt to formulate a five-dimensional theory of relativity. In particular, Klein tried to determine the eigenfrequencies of the harmonic oscillator in this five-dimensional theory; but the attempt to test the theory failed because of mathematical obstacles (Klein did not, for instance, know about Hermite polynomials). It was during these fruitless calculations that Schrödinger's first paper on wave mechanics appeared and at once became the subject of eager discussions in Copenhagen. Klein realized that Schrödinger's theory was a fulfilment of some of his own ambitions, only reached in a much simpler and much more convincing way.

The direction of Klein's thoughts, and their closeness to Schrödinger's approach, may be further illustrated by a letter Pauli wrote to Jordan in April 1926.[189] At that time Schrödinger's second communication had not yet appeared, but Klein must have realized the connection between Schrödinger's non-intuitive Q_1 method and the Debye-Sommerfeld-Runge theory from optics. Pauli writes:

> "Hier noch eine Anmerkung, die ich Herrn Klein verdanke. Der Unterschied zwischen der alten Quantentheorie der Periodizitätssysteme und der auf dem Ansatz (5) basierenden Schrödingerschen Quantenmechanik ist, vom Standpunkt der de-Broglie-Strahlung aus, derselbe wie der zwischen geometrischer Optik und Wellenoptik. Bei kleiner Wellenlänge der de-Broglie-Strahlung kann man nämlich in (5) in bekannter Weise den Ansatz machen
>
> $$\overline{\psi} = e^{i(^1/k)S}$$
>
> Ist S/K gross, so erhält man dann aus (5) nach Debye die Hamilton-Jacobische Differentialgleichung für S. Ueberdies wird in diesem Fall $\overline{\psi}$ nur dann eine eindeutige Ortsfunktion, wenn die Periodizitätsmoduln von S ganze Vielfache von 2π sind. Dies führt auf die bisher übliche $\int p\, dq = nh$ Bedingung, die ja schon von de Broglie selbst vom Standpunkte der geometrischen Optik seines Strahlungsfeldes aus interpretiert wurde.
>
> In Wirklichkeit aber ist S/K im allgemeinen nicht gross, man muss bei (5) bleiben und die Mathematik der Wellenlehre zur Integration dieser Gleichung anwenden."

Klein eventually published his work on a unification of quantum theory and five-dimensional relativity, in which the first KG equation appears, in April 1926.[190]

Following Einstein's fundamental creation of the general theory of relativity, Weyl had sought to extend it so as to furnish an unified explanation of gravitational and electromagnetic phenomena.[191] With the same aim, Theodor Kaluza had in 1921 proposed a five-dimensional version of (general) relativity in which a new space-like coordinate x_0, was introduced in addition to the usual x_1, x_2, x_3 and t coordinates. Later, Kaluza's theory was further developed by Klein[193] and, independently of Klein and Kaluza, also by the Russian physicist H.Mandel.[194] Einstein found the Kaluza-Klein approach promising enough to contribute himself on the five-dimensional theory.[195]

Klein expressed, in accordance with Kaluza, the electromagnetic potentials and the Einsteinian gravitational potentials in a five-dimensional Riemannian space (x_0, x_1, x_2, x_3, t). As to the physical nature of the rather artificially introduced fifth coordinate, Klein proposed that x_0 might be considered as conjugate to the electrical charge in the sense of quantum mechanics. According to Klein, the 'momentum', corresponding to x_0 was expressed as

$$p_0 = \frac{e}{\beta c}$$

It was further suggested that the atomicity of electricity as well as Planck's quantum of action might be interpreted in terms of the five-dimensional theory.[196] But otherwise Klein held x_0 to be unobservable in principle. At about the same time, Fritz London proposed[197] that the fifth coordinate should be related to the spin, so that the spin angular momentum was expressed by the operator

$$d = \frac{h}{2\pi i}\frac{\partial}{\partial x_0} \tag{10.1}$$

However, the physical meaning of the fifth dimension remained obscure. It was indeed understandable when Landau and Iwanenko in Leningrad objected to Klein's "künstlichen Einführung der fünften Koordinate."[198]

In Klein's theory, the motion of electrically charged particles took part along geodesic lines in the five-dimensional world. The equation of motion was interpreted, by means of Hamilton's optical-mechanical analogy, as the ray equation of a wave propagation connected to material particles. Klein imagined "die beobachtete Bewegung als eine Art Projektion auf den Zeitraum von einer Wellenausbreitung, die in einem Raum von fünf Dimensionen stattfindet."[199] By elaborating on these ideas a general equation of motion was found, including wave aspects as well as electromagnetic and gravitational aspects. In the simple electrostatic case, the model of the hydrogen atom, the gravitational terms in the five-dimensional equation become vanishingly small and the following equation was found

$$\Delta U - \frac{1}{c^2}\frac{\partial^2 U}{\partial t^2} - \frac{2e\varphi}{c^2} \cdot \frac{\partial^2 U}{\partial t \partial x_0} + \left(m_0^2 c^2 - \frac{e^2\varphi^2}{c^2}\right) \cdot \frac{\partial^2 U}{\partial x_0^2} = o \qquad (10.2)$$

In here, φ is the electrical potential and U is a wave function associated with the motion of the electron in five-dimensional space. In this wave equation, Planck's constant does not appear originally. It was introduced in connection with an assumed periodicity in x_0:

$$U = \psi\,(x_1, x_2, x_3) \cdot \exp\,\{^{2\pi}/i \quad (^{x}o/h - \nu t)\}$$

If inserted in (10.2), one obtains

$$\Delta\psi + \frac{4\pi^2}{c^2h^2}\,[(h\nu - e\varphi)^2 - m_0^2 c^4)]\,\psi = o \qquad (10.3)$$

That is, the relativistic energy wave equation such as written by Schrödinger five months earlier (this was, of course, unknown to Klein). The general, i.e. time-dependent, wave equation was not explicitly written out by Klein; but it follows immediately from (10.1) if substituting

$$U = \psi(x_1, x_2, x_3, t)\; e^{\frac{2\pi}{ih} x_0}$$

If further $\varphi = -e/r$, we arrive at (6.3). This equation was extensively discussed by Klein in another paper,[200] where he also found the relativistic expressions for charge and current densities, also published by Gordon. In April 1926 Klein further demonstrated that his relativistic equation (10.2) approximates to the usual Schrödinger equation for low velocities, such as to be expected for a reasonable relativistic theory. This is shown most simply if we put $h\nu = m_0c^2 + E$ in (10.2). Then

$$\Delta\psi + 4\pi^2 \left(\frac{E - e\varphi}{hc}\right)^2\psi + \frac{8\pi^2 m}{h^2}(E - e\varphi)\,\psi = 0$$

with the second term vanishing in the classical limit.

As it turns out, Klein's wave equation is, in itself, completely independent of the somewhat speculative introduction of a five-dimensional space. However, since Klein's purpose was primarely to establish a unitary theory of electromagnetism, gravitation and quanta, he did not attach much weight to the four-dimensional wave equation itself (in which gravitation does not appear).[201] In Klein's work, the KG equation was treated in a curiously formal way, not mentioning a word about its physical significance. Thus, Klein did not attempt to find the energy eigenvalues so as to compare his equation with experimental data. This would not have been too difficult a problem after Schrödinger had shown the way in Q_1.

Although Klein's five-dimensional quantum theory was by many physicists considered to be artificial and without proper physical significance, it was rather widely discussed during 1926. Klein was, for instance, invited to Leiden in the spring of 1926 to lecture on the five-dimensional theory, of which Ehrenfest had heard from Copenhagen.[202] In the same year, the young Léon Rosenfeld were among those who, after Schrödinger's first papers had appeared, combined relativity with wave mechanics into a five-dimensional formalism, based on Kaluza's theory.[203] De Broglie, who had learned about the five-dimensional theory from Rosenfeld,[204] joined the trend and worked out his version of five-dimensional quantum theory, only slightly different from Klein's theory.[205] In Leningrad another five-dimensional quantum theory, also it essentially similar to Klein's, was produced by Fock.[206] Remarkably, both Rosenfeld's and Fock's works were made independently of Klein.

The attempts to express quantum mechanics in a world of five dimensions continued for some years, but largely they did not contribute with much of physical interest. After Dirac's electron theory from 1928, the interest in five-dimensional theories faded away.[207]

The application of general relativity to atomic and subatomic physics was in 1926 part of an already established tradition, although Klein was the first one to deal with quantum mechanics in a general relativistic framework. From the very creation of Einstein's gravitational theory, physicists had attempted to apply it to the then atomic model, the Bohr-Sommerfeld atom. This trend was particularly marked in the early twenties, no doubt a product of the intense public interest of which (general) relativity was then a subject.[208] Attempts to reconcile the old quantum theory with general relativity were offered by W.Wilson, T.Wereide, Försterling and others.[209] Even after the emergence of the new quantum mechanics, the trend was followed by some scientists.[210] These attempts invited mathematical jugglery and pretty wild speculations, and they did not contribute to a better understanding of quantum theory. Incidentally, however, one of these attempts, due to Schrödinger, became highly influential to the creation of wave mechanics.[211]

In 1926, and the following years, numerous attempts were made to work out theories of the 'unitary problem', i.e. to formulate a unified picture of gravitation, electromagnetism and quanta, now in the light of the new quantum mechanics. Some of these attempts worked with a five-dimensional theory, most did not. But they all shared the characteristics of their predecessors: They were sites for imaginative formalism and advanced mathematics, but turned out to be almost sterile as regards proper (i.e. empirical) physics. Characteristically, many of the papers on general relativity quantum theory appeared in the *Journal of Mathematical Physics*. Suffice here to mention that Th. de Donder and Fr. van den Dungen from Belgium succeeded to derive the relativistic wave equation from considerations on general relativity dynamics,[212] and that they did so independently of Schrödinger, Klein and Fock. The method of de Donder and van den Dungen was essentially a generalized, covariant form of the variational procedure applied by Schrödinger in Q_1. Other early works on general relativity quantum mechanics were due to Flint and Fisher, Isakson, London, Wiener and Rosenfeld.[213]

The problem of uniting the basic forces of Nature into one grand theory continued to challenge theoretical physicists.[214] It was a dream, too beautiful to be given up. But it has largely remained a dream up to this day.

§ 11. THE EQUATION WITH THE MANY FATHERS

As mentioned earlier, Schrödinger derived the fundamental wave equation in four different ways. These were: 1. By combining de Broglie's formulae with the simple wave equation (unpublished). 2. By means of a variational procedure (Q_1). 3. By means of an extended version of Hamilton's optical-mechanical analogy (Q_2). 4. By applying the quantum mechanical operator prescriptions (Q_4). Of these methods, the first and the last one were used to obtain relativistic equations. That also Schrödinger's methods from Q_2 and Q_1 may easily be modified so as to include relativity, was shown by a number of physicists in 1926. It soon became realized, that if one avoided to go the heavy way around general relativity, then a relativistic generalization of wave mechanics was easy to obtain.

When de Broglie read Schrödinger's first communications on wave mechanics in the spring of 1926, he was fascinated. But he did not regard Schrödinger's theory as a completion of his own ideas. De Broglie disagreed with Schrödinger, not only on the understanding of the wave nature of particles, but also because of the theory's non-relativistic foundation: "In particular, the wave equation which he [Schrödinger] attributed to the wave was not relativistic and I was too convinced of the close liaison between the theory of relativity and wave mechanics to be satisfied with a non-relativistic wave equation."[215]

Accordingly, de Broglie sought for a relativistic generalization of Schrödinger's equations and in July, at a time when Schrödinger's relativistic theory in Q_4 had not yet appeared, he presented complete versions of the Klein-Gordon equations.[216] De Broglie's way to the eigenvalue equation was quite similar to Schrödinger's original unpublished method: if the phase wave of a particle is described by the usual wave equation (5.20), we may substitute the phase velocity with E/p since $E=h\nu$ and $p=h/\lambda$. If furthermore $\psi(\vec{r},t)$ is assumed to be harmonic in the time, $\psi(\vec{r},t)=\psi(\vec{r})\exp(\frac{2i\pi}{h}Et)$, insertion yields

$$\Delta\psi + \frac{4\pi^2 p^2}{h^2}\psi = 0$$

Here p is related to the energy through the relativistic expression

$$c^2\vec{p}^2 = (E - e\phi)^2 - m_0^2c^4$$

From which the Klein-Gordon equation, in the form (6.6) comes out. To obtain the time - dependent equation in its general form, de Broglie simply applied the operator substitutions (5.22) to the relativistic invariant

$$(\frac{E}{c} - \frac{e}{c}\phi)^2 - (\vec{p} - \frac{e}{c}\vec{A})^2 = m_0^2c^2$$

and then obtained (6.3).

That the mere derivation of a relativistic extension of Schrödinger's equation was an easy, not to say a trivial matter, is convincingly shown by Pauli's unpublished derivation from April 1926. Pauli was not, at this occasion, particularly interested in the relativistic Schrödinger equation, which he derived only as a by-product in his proof of equivalence between matrix and wave mechanics.

Right after the appearance of Schrödinger's first quantization paper, many physicists realized that the new wave mechanics, despite of its very different form and outlook, was intimately connected to the already established matrix mechanics. Schrödinger had himself thought so at an early stage, but had at first not been able to figure out the kind of relationship. In February, he wrote to Wien:

"Ich bin mit Geheimrat Sommerfeld von einer innerlich nahen Beziehung überzeugt ... sie muss aber ziemlich tief liegen, denn Weyl, der die Heisenbergsche Theorie sehr gründlich studiert und selbst weiterentwickelt hat, ... sagt, er weiss das Verbindungsglied nicht zu finden."[217]

And in Q_2 Schrödinger admitted in public his failure in finding the relation: "In der *Tendenz* steht der Heisenbergsche Versuch dem vorliegenden ausserordentlich nahe, ... In der Methode ist er so toto genere verschieden, dass es mir bisher nicht gelungen ist, das Verbindungsglied zu finden."[218] However, only a few days later Schrödinger had set the matter straight and had managed to prove a complete mathematical equivalence between the two new quantum theories.[219] Also Carl Eckart from USA established the formal equivalence between matrix and wave mechanics, only a short time after Schrödinger whose proof he did not know about.[220]

Independently, also Pauli had figured out the same thing during one of his frequent travels to Copenhagen. As recalled by Klein:

"Pauli had found it independently a little before Schrödinger's paper appeared. Then Pauli came to Copenhagen. He told me that on the ferry to Gedser he had been walking on the deck, back and forth, and made that up in his head. It was quite clear, so that he told us about it then."[221]

Pauli reported his proof of equivalence in details in a letter to Jordan of April 12.[222] In this interesting letter, Pauli first derived the Klein-Gordon equation in the same way as shown above, and he also showed that this equation gives Schrödinger's eigenvalue equation for small velocities. In Pauli's primary business, the connection between the wave mechanics and the Göttingen theory, he used however only the non-relativistic approximation. In fact, Pauli soon realized that the necessary equivalence between matrix and wave mechanics was not at all possible to establish if one departed from the Klein-Gordon equation. This insight became a major reason to Pauli's lack of confidence in the 'equation with the many fathers' (although Pauli was himself one of these fathers). Pauli's point was expressed in a letter to Wentzel in the beginning of July:

"Die differentialgleichung

$$\Delta\psi - \frac{1}{K^2c^2}(E-E_{pot})^2\psi + \frac{m_0^2c^2}{K^2}\psi = o$$

($K = \frac{h}{2\pi i}$, E = Energie ausschlieslich m_0c^2) hat eine sehr unangenehme Eigenschaft. Sie ist nähmlich nicht selbstadjungiert, die zugehörigen Eigenfunktionen ψ_n sind nicht orthogonal. Daran ist das Glied $\frac{2}{K^2c^2}EE_{pot}$ schuld, das beim ausquadrieren von $(E-E_{pot})^2$ entsteht, wie man sofort sieht, wenn man $\psi_n\Delta\psi_m-\psi_m\Delta\psi_n$ bildet. Wenn man den zusammenhang mit den Matrizen

$$q_{nm} = \int q\psi_n\psi_m dV\ ; \quad P_{nm} = K\int\psi_n\frac{\partial\psi_m}{\partial q}dV$$

beibehalten will, mussen aber die Eigenfunktionen orthogonal sein!"223

In 1926 and 1927 Pauli was much occupied with the relativistic formulation of quantum mechanics, although he did not contribute to this field with publications. It was only in 1934 that Pauli published on the Klein-Gordon equation, and then to revive the then dying second-order equation.[224] Pauli's general lack of faith in the Klein-Gordon equation was reflected in a number of letters. In November 1926 he thus wrote to Schrödinger:

"Beiliegend schreibt Herr Kudar über die schvierigkeit, ich möchte sogar sagen, die Unmöglichkeit, Deine Vorschrift zur Matrizenbildung in relativistischen Fall mit den Multiplikationsregeln im Einklang zu bringen. Überhaupt scheint es mir, dass eine sachgemahe Formulierung der Quantenmechanik bei Berücksichtigung der Relativitätskorrektionen erst möglich sein wird, bis es gelingt, Raum und Zeit als gleichberechtigt zu behandeln. Solange mann genötigt ist, die Feldfunktion ψ, was, ihre Abhängigkeit von die Zeit betrifft, von vornherein nach Sinusfunktionen zu entwickeln, glaube ich kaum, dass die "Wellengleichung" für ψ anders geschrieben werden kann als mit dem linearen Operator

$$\mathcal{D} = \sqrt{1 + \frac{1}{m_0^2 c^2} - \left(\frac{2\pi i}{h}\right)^2 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)}$$

$$(\mathcal{D}(\psi) + V\cdot\psi = E\cdot\psi)$$

das heisst von ∞ hoher Ordnung. Eine solche Wellengleichung ist zwar mathematisch unbequem, aber an sich sinnvoll und auch selbstadjungiert."[225]

Still another, independent version of relativistic wave mechanics was produced by Fock.[226] In the beginning of June, when Fock submitted his paper on the subject, only the first two of Schrödinger's articles on wave mechanics had reached the far-away Leningrad. Fock generalized Schrödinger's variational procedure from Q_1 to include time-dependency as well as relativity. If F is a quadratic function of the first space and time derivatives of ψ, formed from the relativistic Hamilton-Jacobi equation, then the generalized wave equation was obtained from the variation principle

$$\delta \int F \, dx_1 dx_2 dx_3 dt = 0$$

From this, Fock showed, the KG equation comes out. Fock calculated a number of wave mechanical examples, such as Stark effect and Zeeman effect, and in particular he considered the relativistic eigenvalue equation for the hydrogen atom. In this, he completed the work, already communicated in words by Schrödinger, of solving the radial Klein-Gordon equation so as to find the energy eigenvalues. Supported by Schrödinger's mathematics from Q_1, Fock again found the exact Sommerfeld formula, although with the disturbing half-integral quantum numbers. A little later, also Eckart calculated the relativistic fine-structure,[227] although neither did he bother to communicate proofs of his result. More detailed treatments of the radial KG equation for the hydrogen atom were supplied by Epstein[228] and by Brouwer,[229] using mathematical techniques different from Schrödinger's, but reaching the same, unsatisfactory result.

Using one or another of the methods indicated by Schrödinger, the KG equation was also derived by several other physicists during 1926. In addition to the originators, already mentioned, the list includes contributions of Dirac, Gordon, Kudar, Guth, Iwanenko and Landau, Bateman and Epstein.[230] Of these works, it was only Gordon's which turned out to be influential as to the further development of relativistic quantum physics.

SUMMARY

In this work, the principal points under investigation have been:

1. The genesis of Schrödinger's wave equation. Contrary to what has been hitherto assumed, I have shown that Schrödinger's original route to the quantum wave equation was different from any of the versions published in the *Quantisierung* communications. The first, unpublished construction of the Schrödinger eigenvalue equation was much indebted to de Broglie's pioneering ideas from which it rose almost directly.

2. The role of relativity in Schrödinger's theory. In the creative phase of wave mechanics, relativity played a much more decisive role than is usually imagined. Historically, the special theory of relativity was a *conditio sine qua non* for wave mechanics. And more than that: it actively generated the foundation of wave mechanics. The close connection between wave mechanics and relativity was emphasized by e.g. Haas, who showed that the fundamental relativistic formulae may be derived on a purely classical basis if only combined with the idea of matter waves in de Broglie's sense.[231]

3. The hydrogen atom as a crucial case for wave mechanics. The experimental and theoretical knowledge of the hydrogen spectrum was decisively important to the way in which wave mechanics emerged. This case also played, although less decisively, a key role in the first phase of matrix mechanics. The all *too* successful explanation of the hydrogen spectrum given by Sommerfeld's theory, was in particular a puzzle for the early quantum mechanics and caused, more than anything else, quantum mechanics to appear in a non-relativistic form. Viewed with hindsight, this was undoubtedly an advantageous accident as the entire development and interpretation of quantum mechanics, such as

it took place in 1926-27, would not have been possible if grounded on a basic equation of the Klein-Gordon type and not on the first-order, non-relativistic Schrödinger type.

4. <u>The significance of mathematics in the birth of wave mechanics</u>. In fabricating quantum mechanics, the crucial role of physicists' knowledge to advanced mathematical analysis was manifest at many occasions. The basic barrier to wave mechanics was of a mathematical, not a physical sort. It was only Schrödinger's concentrated study of differential equations that turned the de Broglie-Schrödinger hypothesis into a powerful and convincing physical theory. If not by other reasons, de Broglie's unsatisfactory mathematical knowledge prevented him in creating a proper wave mechanics. Also the route followed by Heisenberg was in no small measure determined by what appeared to be mathematically manageable. If the hydrogen atom, not the anharmonic oscillator, had been chosen as the prime example for matrix mechanics, the early history of quantum mechanics would surely have been much different.

5. <u>Oskar Klein's almost-discovery of wave mechanics</u>. Although Schrödinger was the sole inventor of wave mechanics, there were a few other attempts tending towards a similar understanding. The most interesting of these attempts was the one due to Oskar Klein who, under more fortunate circumstances, might perhaps have obtained a wave mechanics prior to Schrödinger. However, Klein's approach was largely ineffective, not least because of its ambitious but premature association with general relativity. Although the most recent development in theoretical physics (such as the 'Grand Unified Theory' of Weinberg a.o.) may be seen as a justification of Klein's approach, in the twenties it was bound to be a blind alley.

NOTES AND REFERENCES

1. E.Schrödinger, "Zur Einsteinschen Gastheorie," Phys. Zeits., 27 (1926), 95-101 (received 15 december 1925); p. 95. Although submitted for publication one and a half month before Schrödinger's first paper on wave mechanics, it was only issued at 1 March 1926, at about the same date that the wave mechanical paper was published.

2. The most detailed expositions of de Broglie's theory are those given by Gerber and Kubli. J.U.Gerber, "Geschichte der Wellenmechanik," Arch. Hist. Ex. Sci., 5 (1969), 349-416. F.Kubli, "Louis de Broglie und die Entdeckung der Materiewellen," Arch. Hist. Ex. Sci., 7 (1970/71), 26-68. F.Kubli, "A propos du 50e anniversaire de la mécanique ondulatoire," Revue d'Hist. Sci., 28 (1975), 97-112. F.Kubli, "La Thèse de 1924," pp. 19-36 in Louis de Broglie. Sa conceptions du monde physique, Paris, 1973. See also E.MacKinnon, "De Broglie's Thesis: a Critical Retrospective," Am. J. Phys., 44 (1976), 1047-1055. H.A.Medicus, "Fifty Years of Matter Waves," Phys. Today, 27 (1974), 38-45.

3. Recherches sur la théorie des quanta, Paris 1924. The thesis was presented on November 29, 1924. It was also published, under the same title, in Annales de Physique, 3 (1925), 22-128. A reedition of the thesis was published in Paris in 1963. In the following, we refer to the 1963 edition.

4. Ibid., p. 20.

5. Ibid., p. 33.

6. Ibid., p. 43

7. The famous 'Planck-Einstein equation' $E=h\nu$ is first contained in Einstein's "Über einen die Erzeugung und die Verwandlung des Lichts betreffenden heuristischen Gesichtspunkt," Ann.d.Phys., 17 (1905), 132-148; $p={}^{h}/\lambda$ first appears in "Zur Quantentheorie der Strahlung," Phys.Zeits., 18 (1917), 121-128.

8. This myth has been propounded by such prominent physicists as Dirac and Born, cf: "De Broglie's ideas applied only to free electrons and Schrödinger was faced with the problem of modifying de Broglie's equation to make it apply to an electron moving in a field, in particular, to make it apply to electrons in atoms." P.A.M.Dirac, The Development of Quantum Theory, New York 1971, p. 37. "Schrödinger --- established the general wave equation which holds not only

for free electrons but also for those bound in atoms." M.Born, Experiment and Theory in Physics, Cambridge 1943; p. 22.

9. It is, therefore, a little disturbing often to hear about 'de Broglie's wave equation', such as used, for instance, by Dirac in his memoirs on the birth of wave mechanics (see § 7).

10. Note 3, p. 53.

11. See note 13, below.

12. For a further appraisal of the role of relativity in de Broglie's work, see M.A. Tonnelat, "L'influence de la relativité sur l'œuvre de Louis de Broglie," pp. 37-52 in Louis de Broglie (note 2).

13. L. de Broglie, Albert Einstein, Publications de l'Institut Henri Poincaré, Paris 1955; p. 16.

14. note 2 (1970/71), pp. 54-57.

15. For Schrödinger's intellectual and professional background, see W.T.Scott, Erwin Schrödinger. An Introduction to his Writings, Amherst (Mass.), 1967.

16. E.Schrödinger, "Quantisierung als Eigenwertproblem, Erste Mitteilung," Ann. d. Physik, 79 (1926), 361-376 (received 27 January); p. 373. This paper is in the following referred to as Q_1.

17. F.Hund, "Irrwege und Hemmungen beim Werden der Quantentheorie," pp. 1-10 in H.P.Dürr (ed.), Quanten und Felder, Braunschweig 1971. Hund has continued his speculations about possible alternative ways to quantum mechanics in "Hätte die Geschichte der Quantentheorie auch anders ablaufen können?" Phys. Blätter, 32 (1975), 29-35.

18. According to AHQP interview of 17 October 1962. See M. Jammer, The Conceptual Development of Quantum Mechanics, New York 1966, p. 223.

19. M. Born, My life. Recollections of a Nobel Laureate, London 1978; p. 226.

20. For this question, cf. the argumentation of N. Russell Hanson, "Are Wave Mechanics and Matrix Mechanics Equivalent Theories?" pp. 401 - 428 in H.Feigl and G.Maxwell (eds.), Current Issues in the Philosophy of Science, New York 1961. Also ch. 8 in N.R.Hanson, The Concept of the Positron, Cambridge 1963.

21. Cf. Jammer (note 18), p. 248.

22. "Je me rapelle vivement ses [i.e. Langevin's] explications enthousiastes à ce sujet, mais je me souviens aussi que c'est seulement avec des hésitations et des doutes que je suivais ses développements." A.Einstein, "Paul Langevin," La Pensée, no. 12 (1947), 13-14.

23. A.Einstein, "Quantentheorie des einatomigen idealen Gases," Sitzungsber. Preuss. Akad. Wiss., 1925, 3-14.

24. L. de Broglie, "A Tentative Theory of Light Quanta," Phil. Mag., 47 (1924), 446-458.

25. "Die ganze Sache [wäre] sicherlich nicht jetzt und vielleicht nie entstanden (ich meine, nicht von meiner Seite), wenn mir nicht durch Ihre zweite Gasentartungsarbeit auf die Wichtigkeit der de Broglieschen Ideen die Nase Gestossen worden wäre." Letter, Schrödinger to Einstein, 23 April 1926. K.Przibram (ed.), Briefe Zur Wellenmechanik, Wien, 1963; p.24.

26. AHQP interview of 8 January 1963. See Jammer (note 18), p. 258 and Gerber (note 2), p. 390. Here, as elsewhere in this text AHQP stands for Archive for History of Quantum Physics (cf. note 170). For cooperation and permission to use the Archive material, I am indebted to Erik Rüdinger, the Niels Bohr Institute, Copenhagen.

27. P.A.Hanle, "The Coming of Age of Erwin Schrödinger: His Quantum Statistics of Ideal Gases," Arch. Hist. Ex. Sci., 17 (1977), 165-192. Also Gerber (note 2) and L.A.Wessels Schrödinger's Interpretation of Wave Mechanics, Dissertation, Un. Wisconsin, 1975. Wessels' account of Schrödinger's route to wave mechanics will appear in an article in the December issue of Stud. Hist. Phil. Sci. I am indebted to Linda Wessels for sending me a copy of her manuscript.

28. Note 1, p.97. The impact of Einstein's gas theory upon de Broglie's and Schrödinger's works, and the importance of Schrödinger's mid-December paper in particular, has been strongly argued by Martin Klein. See "Einstein and the Wave-Particle Duality," The Natural Philosopher, 3 (1964), 3-49.

29. AHQP interview of 5 april 1962. Also the 80 years anniversary article "Peter J.W.Debye: An interview," Science, 145 (1964), 554-559.

30. Ibid., p.554. Later in the interview: "It was in the same year that he published his paper, because there was only a few months between his talk and his publication."

31. In the AHQP interview, Debye is very certain about this point. Medicus' suggestion (note 2, p.42), that Schrödinger had read de Broglie's thesis before it appeared in the Annales, is then mistaken.

32. F.Bloch, "Heisenberg and the Early Days of Quantum Mechanics, "Phys. Today," December 1976, 23-27; p.23.

33. Letter, Schrödinger to Einstein, 3 November 1925. See P.A.Hanle, "Schrödinger's Reaction to de Broglie's Thesis," Isis, 68 (1977), 606-609. Also P.A.Hanle, "The Schrödinger-Einstein Correspondence and the Sources of Wave Mechanics," Am. J. Phys., 47 (1979), 644-648.

34. E.Schrödinger, "Über eine bemerkenswerte Eigenschaft der Quantenbahnen eines einzelnen Elektrons," Zs. f. Phys., 12 (1922), 13-23.

35. V.V.Raman and P.Forman, "Why was it Schrödinger who Developed de Broglie's Ideas?" Hist. Stud. Phys. Sci., 1 (1969), 291-314.

36. Note 33.

37. Ibid.

38. Quoted from note 35, p. 313.

39. Note 27, p. 55.

40. AHQP. Part of this letter has been quoted (in English translation) by A.Hermann, "Erwin Schrödinger," pp. 217 - 223 in C.C.Gillispie (ed.), Dictionary of Scientific Biography, vol. 12, New York 1975. The letter, which is in Schrödinger's handwriting is, as are all of his handwritten material, very difficult to read. Wessels' reproduction of parts of the same letter (note 27, p.356) is inaccurate at several points. For assistance in deciphering Schrödinger's handwriting, I am indebted to Bernhelm Booss. Bessel's differential equation, mentioned by Schrödinger, is of the form

$$\frac{d^2U}{dx^2} + \frac{1}{x}\frac{dU}{dx} + \left(1 - \frac{k^2}{x^2}\right) U = 0$$

it may be considered as a special case of Laplace's differential equation, the one appearing in Schrödinger's treatment of the hydrogen atom (see eq. (8.8) with $\delta_0=0$, $\delta_1=1$, $\varepsilon_0=1$ and $\varepsilon_1=-k^2$).

41. Q_1, p. 374. See also this article, § 6.

42. L. de Broglie, "Sur un théoreme de Bohr," Comptes Rendus, 179 (1924), 676.

43. On this subject there is much information to obtain from Jammer (note 18) and from E.T.Whittaker, A History of the Theories of Aether and Electricity, vol. 1-2, London 1953. Cf. also the monograph by G.W.Series, The Spectrum of Atomic Hydrogen, Oxford 1957, which calls particular attention to the development following Dirac's relativistic theory.

44. Cf. J.L.Heilbron and T.S.Kuhn, "The Genesis of the Bohr Atom," Hist. Stud. Phys. Sci., 1 (1969), 211-290, esp. p. 264.

45. Cf. Jammer (note 18), p. 89.

46. This is the value reported by Sommerfeld in Atombau und Spektrallinien, Braunschweig 1924.

47. Cf. J.L.Heilbron, "The Kossel-Sommerfeld Theory and the Ring Atom," Isis, 58 (1967), 451-482.

48. Cf. P.Forman, "The Doublet Riddle and Atomic Physics circa 1924," Isis, 59 (1968), 156-174; p. 163.

49. J.H. Van Vleck, "Travels with Dirac in the Rockies," pp. 7-16 in A.Salam and E.P.Wigner (eds.), Aspects of Quantum Theory, Cambridge 1972; p. 9.

50. R.Kronig, "The Turning Point," pp. 5-39 in M.Fierz and V.F.Weisskopf, (eds.) Theoretical Physics in the Twentieth Century. A Memorial Volume to Wolfgang Pauli, New York 1960; p. 9.

51. E.Lau, "Über die Frage der Feinstruktur ausgewählter Spektrallinien," Phys.Zs., 25 (1924), 60-68. E.Gehrcke and E.Lau, "Über das Wasserstoffspektrum," Ann.d.Phys., 76 (1925), 673-679. L.Janicki, "Über die Balmerserie des Wasserstoffs," Ann.d.Phys., 76 (1925), 561-566. L.Janicki and E.Lau, "Zur Feinstrukturfrage," Zs.f.Phys., 35 (1925-26), 1-6.

52. P.H.van Cittert, "Zur Messung der Feinstruktur der Wasserstofflinien mit der Lummer-Gerchke-Platte," Ann.d.Phys., 77 (1925), 372-380. F.Paschen, "Die relativistische Feinstruktur von Spektrallinien," Ann.d.Phys., 82 (1927), 689-696.

53. G.Hansen, "Die Feinstruktur der Balmerlinien," Ann.d.Phys., 78 (1925), 558-600.

54. W.V.Houston, Astrophys. Journal, 64 (1926), 81. N.A.Kent, L.B.Taylor and H.Pearson, "Doublet Separation of Fine Structure of the Balmer Lines of Hydrogen," Phys. Rev., 30 (1927), 266-283. Also for the He^+ spectrum similar disagreements were reported. Uhlenbeck and Goudsmit, for instance, called attention to a component of the 4686 line which, in the old notation, was due to the 'forbidden' transition $4_1 \rightarrow 3_1$; the same thing was pointed out by Slater. S.Goudsmit and G.Uhlenbeck, "Opmerking over de Spectra van Waterstof en Helium," Physica, 5 (1925), 266-270, (August). J.C.Slater, "Interpretation of the Hydrogen and Helium Spectra," Proc. Nat. Acad. Sci., 11 (1925), 732-738 (communicated 16 November 1925).

55. M.Bronstein, "Über die Bewegung eines Elektrons im Felde eines festen Zentrums mit Berücksichtigung der Massenveränderung bei der Ausstrahlung," Zeits. f. Phys., 35 (1926), 863-882. "Zur Theorie der Feinstruktur der Spektrallinien," Zeits. f. Phys., 37 (1926) 217-224.

56. J.Kudar, "Bemerkung zur Arbeit des Herrn M.Bronstein," Zeits. f. Phys., 37 (1926), 861-862.

57. A.H.Bucherer, "Die Feinstruktur der Wasserstofflinien," Zeits. f. Phys., 37 (1926), 395-404.

58. For these physicists, and their conflict with quantum theory and Einsteinian relativity, see A.D.Beyerchen, Scientists under Hitler: Politics and the Physics Community in the Third Reich, Yale 1978. The Lenard-inspired critique of relativity was predominantly a German affair, but it was also found outside Germany. Thus, Vallarta in USA departed from Lenard's objections to relativity and claimed that neither the special nor the general theory of relativity could properly account for the spectral fine-structure; see M.S.Vallarta, "Bohr's Atomic Model from the Standpoint of General Relativity," Phys.Rev., 25 (1925), 582.

59. Cf. A.H.Bucherer, "Gravitation und Quantentheorie," Ann. d. Phys., 68 (1922), 1-10 and 546-551. Bucherer was a theoretical physicist of the old school, his major work being in the classical theory of electrons; in 1904 he had produced a theory of the moving electron, being alternative to Abraham's as well as to Lorentz'. In the history of physics Bucherer is, curiously, most known as an experimentalist, namely for his early experiments on the specific charge of high-speed electrons (A.H.Bucherer, "Messungen an Bequerelstrahlen. Die experimentelle Bestätigung der Lorentz-Einsteinschen Theorie," Phys.Zeits., 9 (1908), 755-762.)

Ironically, although Bucherer in 1908 and in most of his career rejected the theory of relativity, these experiments provided the first experimental support for relativistic dynamics.

60. See E.Gehrcke, Kritik der Relativitätstheorie. Gesammelte Schriften über absolute und relative Bewegung, Berlin 1924. In accordance with Lenard's and Stark's attacks on Einstein, Gehrcke claimed that the experimentally verified formulae of the theory of relativity were not at all due to Einstein, but their priority belonged to earlier physicists of German -and Aryan- birth.

61. Forman (note 48) and D.Serwer, "Unmechanischer Zwang: Pauli, Heisenberg, and the Rejection of the Mechanical Atom, 1923-1925," Hist.Stud.Phys.Sci., 8 (1977). 189-256.

62. R.A.Millikan and I.S.Bowen, "Some Conspicouos Successes of the Bohr Atom and a Serious Difficulty," Phys.Rev., 24 (1924), 223-228.

63. Ibid., p.227.

64. R.A.Millikan and I.S.Bowen, "A Possible Reconciliation of Bohr's Interpenetration Ideas with Sommerfeld's Relativistic Treatment of Electron Orbits," Phil.Mag., 49 (1925), 923-935. For Bohr's theory of penetrating orbits, see H.Kragh, "Niels Bohr's Second Atomic Theory," Hist. Stud.Phys.Sci., 10 (1979), 123-186.

65. Ibid., p.925.

66. Ibid., p.935.

67. Cf. Forman (note 48), p.169.

68. O.Oldenberg, "Zur Feinstruktur der Balmerserie," Ann. d. Phys., 67 (1922), 69-72. "Die Feinstruktur der roten Wasserstofflinie und ihr Zeemaneffekt," Ibid., 253-277.

69. K.Försterling and G.Hansen, "Zeemaneffekt der roten und blauen Wasserstofflinie," Zs.f.Phys., 18 (1923), 26-33.

70. A.Sommerfeld and A.Unsöld, "Über das Spektrum des Wasserstoffs," Zs.f.Phys., 36 (1926), 259-275; p. 268.

71. Cf. Forman (note 48), p.163.

72. T.S.Kuhn, The Structure of Scientific Revolutions, New York 1969.

73. Note 54.

74. Ibid.

75. Cf. Forman (note 48), p.173 and Jammer (note 18), p.95.

76. Note 70.

77. Ibid., p.275.

78. Note 54, p.282.

79. B.L.van der Waerden, "Exclusion Principle and Spin," pp. 199-244 in Pauli memorial volume (note 49). Kronig (note 49). S.Goudsmit, "Entdeckung der Elektronspins," Phys.Blätter, 21 (1965), 445-453.

80. Apart from a little convincing argument from classical electron theory where Abraham had in 1903 shown that the gyromagnetic ratio of a rotating sphere with surface charge is exactly twice the ratio for orbital revolution. For details, see A.I.Miller, "A Study of Henri Poincaré's 'Sur la dynamique de l'éléctron'," Arch.Hist.Ex.Sci., 10 (1973), 207-328.

81. That Heisenberg originally started out with the hydrogen atom, not with the anharmonic oscillator, is confirmed by Heisenberg in an AHQP interview of 1963. See E.MacKinnon, "Heisenberg, Models, and the Rise of Matrix Mechanics," Hist.Stud.Phys.Sci., 8 (1977), 137-187, on pp.162-164. See also C.P.Enz, "W.Pauli's Scientific Work," pp.766-799 in J.Mehra (ed.), The Physicist's Conception of Nature, Dordrecht 1973, on p.772.

82. W.Pauli, "Über das Wasserstoffspektrum vom Standpunkt der neuen Quantenmechanik," Zs.f.Phys., 36 (1926), 336-363 (received 17 January 1926). Translated in B.L.van der Waerden, Sources of Quantum Mechanics, Amsterdam 1967, pp.387-415.

83. J.H. Van Vleck, "My Swiss Visits of 1906,1926 and 1930," Helvetica Physica Acta, 41 (1968), 1234-1237; p.1234.

84. As quoted from van der Waerden (note 82), p.58.

85. W.Heisenberg, "Erinnerungen an die Zeit der Entwicklung der Quantenmechanik," pp.40-47 in Pauli memorial volume (note 49); p.43.

86. Pauli's reputation as a committed relativist stemmed particularly from his early exposition of the theory of relativity. W.Pauli, "Relativitätstheorie," Encyklopädie der Math. Wissenschaften, vol. V 19 (Leipzig 1921). Translated by G.Field, Theory of Relativity, Oxford 1958. For an appraisal of Pauli's commitment to relativity, see V.Bargmann, "Relativity," pp.187-198 in Pauli memorial volume (note 49). Pauli's 'relativistic' stand in the debate over doublet spectra is exposed in Forman (note 48), Serwer (note 61) and Jammer (note 18).

87. Van der Waerden (note 82) and J.H.Van Vleck (note 94).

88. Note 82, p. 361.

89. This is seen: $E_k = m_0c^2 \left(1 + \frac{p^2}{m^2c^2}\right)^{\frac{1}{2}} - mc^2 \approx E_{o,k} + E_1$

where $E_{o,k} = \frac{p^2}{2m}$ and $E_1 = -(2mc^2)^{-1} \left(\frac{p^2}{2m}\right)^2$

i.e. $E_1 = -(2mc^2)(E_o - U)^2 = -(2mc^2)(E_0^2 - 2E_oU + U^2)$

with $U = -e^2/r$ this gives the expression in the text.

90. P.A.M.Dirac, "Quantum Mechanics and a Preliminary Investigation of the Hydrogen Atom," Proc. Roy. Soc. (London), A110 (1926), 561-579 (received 22 January 1926). Most of this paper is reproduced in van der Waerden's collection (note 82), however not the part dealing with the hydrogen spectrum.

91. P.A.M.Dirac, "Recollections of an Exciting Era," pp. 109-146 in C.Weiner (ed.), History of Twentieth Century Physics, New York 1977; p. 130.

92. Letter, Heisenberg to Dirac, 20 November 1925. Quoted from Dirac, op.cit. p. 125.

93. G.Wentzel, "Die mehrfach periodischen Systeme in der Quantenmechanik," Zs. f. Phys., 37 (1926), 80-94 (received 27 March 1926).

94. J.H.Van Vleck, "Central Fields in Two Vis-a-Vis Three Dimensions: an Historical Divertissement," pp. 26-37 in W.C.Price et.al.(eds.), Wave Mechanics: The First Fifty Years, New York 1973; p.31.

95. Letter, Schrödinger to Lorentz, 6 June 1926. Quoted from Przibram (note 25), p.59.

96. See also H.Kragh, "The Genesis of Dirac's Relativity Theory of Electrons," (to be published).

97. Letter, Pauli to Wentzel, 5 July 1926 (AHQP).

98. See note 96.

99. L.H.Thomas, "The Motion of the Spinning Electron," Nature, 117 (February 1926), 514. A more detailed account appeared in L.H.Thomas, "The Kinematics of an Electron with an Axis," Phil. Mag., 3 (1927), 1-22. See also J.Frenkel, "Die Elektrodynamik des rotierendes Elektrons," Zs. f. Phys., 37 (1926), 243-262.

100. Letter, Kramers to Kronig, 26 February (AHQP).

101. W.Heisenberg and P.Jordan, "Anwendung der Quantenmechanik auf das Problem der anomalen Zeemaneffekte," Zs. f. Physik, 37 (1926), 263-277 (received 16 March 1926).

102. M.Born, W.Heisenberg and P.Jordan, "Zur Quantenmechanik, II," Zs. f. Phys., 35 (1926), 557-615 (received 16 November 1925).

103. AHQP. Quoted from Serwer (note 61) p. 251. See also the other quotations from Heisenberg's letters to Goudsmit and Pauli in the same article.

104. Letter, Heisenberg to Goudsmit, 19 February 1926 (AHQP).

105. Ibid.

106. C.F.Richter, "The Spinning Electron in Hydrogen-like Spectra," Phys.Rev., 28 (1926), 849 (presented 17 June 1926).

107. Note (95).

108. Note (101), p. 274.

109. Note (94).

110. E.Schrödinger, "Quantisierung als Eigenwertproblem, Zweite Mitteilung," Ann. der Physik, 489-527, 79 (1926), 489-527 (received 23 February 1926). In the following called Q_2.

111. Jammer, (note 18), p. 261.

112. Q_1, p. 372.

113. Q_2, p. 489.

114. Ibid.

115. Note 27.

116. E.Schrödinger, Abhandlungen zur Wellenmechanik, Leipzig 1927; preface dated November 1926.

117. A.Hermann, "Erwin Schrödinger - Eine Biographie," pp. 173 - 192 in A.Hermann (ed.), Die Wellenmechanik (Dokumente der Naturwissenschaft, Abteilung Physik, Band 3), Stuttgart 1963.

118. A.Hermann, Die Jahrhundertwissenschaft, Stuttgart 1977; p. 84. Hermann writes: "In Februar 1926, nach seiner ersten Mitteilung über Quantisierung als Eigenwertproblem, stiess Schrödinger dann auf die fast einhundert Jahre alten Arbeiten der irischen Mathematikers William Rowan Hamilton.--- Die Hamiltonsche Theorie war nicht, wie Historiker bisher immer gemeint hatten, der Zugang zur Wellenmechanik. Die alten Arbeiten waren vielmehr eine "Überraschung" für Schrödinger, als er seine Theorie schon in den Grundlagen fertig hatte."

119. See F.Klein, Gesammelte Mathematische Abhandlungen, II, Berlin 1922, pp. 601-602. Probably, however, Schrödinger was unaware of Klein's contributions to Hamilton's analogy until January 1926. In a footnote in Q_2, p. 490, Schrödinger expresses his debt to Sommerfeld for having called attention to Klein's works.

120. Microfilmed by AHQP. See note 35, p. 303.

121. N_2, see § 8.

122. Note 2, (1970/71 and 1975). As well known to physicists, Schrödinger's substitution

$S = \frac{h}{2\pi} \ln \psi$ (or $S = \frac{ih}{2\pi} \ln \psi$) is essentially the one applied in the so-called WKB approximation. This method, first worked out in 1926, establishes the Bohr-Sommerfeld theory as the classical limit of Schrödinger's wave mechanics. See Jammer (note 18), pp. 277-279 or Whittaker (note 43), pp. 280-283.

123. A.Sommerfeld and I.Runge. "Anwendung der Vektorrechnung auf die Grundlagen der geometrischen Optik," Ann. d. Phys. 35 (1911), 277-298.

124. Q_2, p. 496. Schrödinger called the eikonal equation for the "Hamiltonsche Gleichung".

125. In 1915. Quoted from S.Goldberg, "Max Planck's Philosophy of Nature and his Elaboration of the Special Theory of Relativity," Hist. Stud. Phys. Sci., 7 (1976), 125-161, p. 149.

126. Letter, E.Fues to T.S.Kuhn, 24 July 1963 (AHQP).

127. N_2, see § 8.

128. Jammer (note 18), Kubli (note 2), Gerber (note 2), Scott (note 15). A good, elementary exposition of the Q_2 method may also be found in W.H.Cropper, The Quantum Physicists, Oxford 1970. For the history of Hamilton's analogy and its use in wave mechanics, see S.Mandelstam and W.Yourgraw, Variational Principles in Dynamics and Quantum Theory, London 1958.

129. In Q_2 Schrödinger used a non-Eucledian metric, based on the kinetic energy T of the system considered. In Schrödinger's metric, which was taken over from H.Hertz, the line element is given by $ds = \sqrt{2T}\,dt$, or, otherwise expressed, $ds^2 = m \sum dq_k^2$. By this reason, all of Schrödinger's equations in Q_2 appear in a different form than those usually seen. The wave equation, for instance, does not contain the mass, but reads $\Delta\psi + \frac{8\pi^2}{h^2}(E-U) = 0$. For our purpose, we shall transcribe Schrödinger's formulae in usual, Eucledian metric.

130. Q_2, p. 497.

131. E.Schrödinger, "Über das Verhältnis der Heisenberg-Born-Jordanschen Quantenmechanik zu der meinen," Ann. der Physik, 79 (1926), 734-756 (received 18 March 1926).

132. M.Born and N.Wiener, "Eine neue Formulierung der Quantengesetze für periodische und nichtperiodische Vorgänge," Zs. f. Phys., 36 (1926), 174-187 (received 5 January 1926).

133. E.Schrödinger, "Quantisierung als Eigenwertproblem, Vierte Mitteilung," Ann. d. Phys., 81 (1926), 109-139 (received 21 June 1926). In the following called Q_4.

134. Q_1, p. 361.

135. Q_1, p. 372.

136. Note 131, p. 735.

137. 'Atomystik' was the nickname for the new quantum theory, particularly used by the Munich experimentalists. See W.Heisenberg, "Theory, Criticism and a Philosophy," pp. 31-47 in From a Life in Physics, IAEA Bulletin, 1969.

138. Born described Schrödinger's programme in quantum mechanics as being the hope for "den Weg zur klassichen Physik der anschaulich erfassbaren Vorgänge zurückzufinden,"
M.Born, "Erwin Schrödinger. Obituary," Phys. Blätter, 17 (1961), 85-87.

139. Letter, Schrödinger to Planck, 26 February (AHQP). Schrödinger's reference to Sommerfeld alludes to the preface of Sommerfeld's classic, Atombau und Spektrallinien, where it is said: "Was wir heuzutage aus der Sprache der Spektren heraus hören, ist eine wirkliche Sphärenmusik des Atoms,.... Alle ganzzahligen Gesetze der Spektrallinien und der Atomistik fliessen letzten Endes aus der Quantentheorie. Sie ist das geheimnisvolle Organon, auf dem die Natur die Spektralmusik spielt und nach dessen Rhythmus sie den Bau der Atome und der Kerne regelt."
(Fourth edition, Braunschweig 1924).

140. A.I.Miller, "Visualization Lost and Regained: The Genesis of the Quantum Theory in the Period 1913-27," pp. 74-102 in J.Wechsler (ed.), On Aesthetics in Science, Cambridge (Mass.), 1978; on p. 86.

141. E.Schrödinger, "An Undulatory Theory of the Mechanics of Atoms and Molecules," Phys. Rev., 28 (1926), 1049-1070; p. 1070.

142. Q_1, p. 372.

143. Q_1, pp. 373-374. Cp. Schrödinger's letter to Wien, quoted in § 2. See also the discussion in Wessels (note 27).

144. Q_2, p. 497.

145. "Ich habe mich hier auf den Fall der klassischen Mechanik beschränkt, da mir die relativistisch-magnetische Verallgemeinerung noch nicht genügend abgeklärt scheint. Dass aber auch für sie der vollkommene Parallelismus der beiden neuen Quantentheorien bestehen bleiben wird, ist kaum zu bezweifeln." Note 131, p. 750. "... es ist ja ganz

sicher, dass sich prinzipiel an der Begründung der Auswahlregeln nichts ändern wird, auch wenn das 'spinning electron-' in der Wellenmechanik seinen richtigen Platz gefunden haben wird." Letter, Schrödinger to Wentzel, 11 May 1926 (AHQP).

146. Cf. note 96.

147. E.Schrödinger, "Quantisierung als Eigenwertproblem, Dritte Mitteilung," Ann. de. Phys., 80 (1926), 437-490; p. 439 (received 10 May 1926). In the following called Q_3.

148. Q_2, p. 514.

149. N_3, cf. § 8.

150. Q_3, p. 476.

151. Ibid.

152. In relativistic quantum mechanics, the charge density is expressed as $\rho \sim \psi^* \frac{\partial \psi}{\partial t} - \frac{\partial \psi^*}{\partial t} \psi \sim \mathrm{Im}(\psi \frac{\partial \psi^*}{\partial t})$

153. Q_4, 132.

154. Quoted from Hermann (note 111), p. 174.

155. They do cover interviews with *Frau* Schrödinger. These are, however, not very illuminating as to the genesis of wave mechanics.

156. "Obituary. Erwin Schrödinger," Nature, 189 (1961), 356. "The Evolution of the Physicist's Picture of Nature," Scientific American, 208 (1963), 45-53. The Development of Quantum Theory, New York 1971. "Recollections of an Exciting Era," pp. 109-146 in C.Weiner (ed.), note (91). "Methods in Theoretical Physics," pp. 21-28 in From a Life in Physics, IAEA Bulletin, 1969. "Hopes and Fear," Eureka, no.32 (1969), 2-4.

157. Ibid. (1977), pp. 136-137.

158. See Jammer (note 18), p. 257; Hermann (note 117), p. 180; Scott (note 15), p. 51.

159. Forman and Raman regard anecdotes, such as Dirac's, as historical allegories, whose social function is to convey certain morales about science and scientists' conduct. Like the myth, scientists' anecdotes purport to be historical but are, in fact, only indirectly related to historical reality. Their function is social and ideological, not scientific, In another

context, Forman has analysed the role of myths and anecdotes in the social culture of science. See P.Forman, "The Discovery of the Diffraction of X-Rays by Crystals; A Critique of the Myths," Arch.Hist.Ex.Sci., 6 (1969), 38-71.

160. See note 8 (1971), p. 40.

161. Interview with D.M.Dennison, 30 January 1964. AHQP transcript.

162. Note 128, p. 114.

163. It is not in the AHQP material. Also it is not among the Schrödinger material, deposited in Vienna, cf. note 171.

164. See note 126.

165. Letter, E.Fues to T.S.Kuhn, Summer 1963 (AHQP).

166. Note 139.

167. Letter, E.Schrödinger to W.Wien, 22 February 1926 (AHQP).

168. Letter, Schrödinger to Weyl, 1 April 1931. Quoted from Gerber (note 2).

169. E.Schrödinger, "Sur la théorie relativiste de l'éléctron et l'interpretation de la mécanique quantique," Ann. Inst. Poincaré, 2 (1932), 269-310; p. 287.

170. In the AHQP archive system, Schrödinger's notebooks are filed under the numbers N_1: (40.5), N_2: (40,5), N_3: (40,6), N_4: (40,6), N_5: (40,7), N_6: (41,1.1). See T.S.Kuhn, J.L.Heilbron, P.Forman and L.Allen, Sources for History of Quantum Physics, Philadelphia 1967.

171. The five notebooks on relativistic quantum mechanics are, together with other Schrödinger materials, deposited at the Zentralbibliothek der Physikalischen Institute der Universität Wien. The director of the library, Dr. Wolfgang Kerber, has kindby informed me that the notebooks are most probably written after 1928. This is also the opinion of Paul Hanle, who has studied Schrödinger's material in Vienna. The five notebooks seem then to deal with Dirac's electron theory, which in the period 1930-34 was a major reasearch topic for Schrödinger.

172. Schrödinger acknowledged his debt to Weyl in Q_1, p. 363.

173. L.Schlesinger, Einführung in die Theorie der gewönlichen Differentialgleichungen auf funktionentheoretischer Grundlage, Leipzig 1900 (third, revised ed., Leipzig 1922). The relevant parts appear particularly on pp. 257-266 (third ed.).

174. For the mathematical development of solutions to the Laplace equation and related differential equations, see A.Schlissel, "The Development of Asymptotic Solutions of Linear Ordinary Differential Equations, 1817-1920," Arch. Hist. Ex. Sci., 16 (1976/77), 307-378.

175. D.Hilbert and R.Courant, Methoden der mathematischen Physik, Berlin 1924. For the history of this classic and its impact on theoretical physics in the twenties, see C.Reid, Courant in Göttingen and New York, New York 1976.

176. Laguerre polynomials were used extensively by Schrödinger in Q_3, when dealing with the Stark effect. From notes in Q_2 (p. 518) and Q_3 (p. 479) it appear that Schrödinger became only aware of the connection of Laguerre polynomials with the radial eigen-functions of the hydrogen atom after having finished Q_1.

177. Treatments of the analysis of the Klein-Gordon equation are seldom found in modern textbooks on quantum mechanics. An exception is L.I.Schiff, Quantum Mechanics, New York 1955 (p. 318 ff). Detailed analyses, being in accordance with Schrödinger's original calculations, may be found in A.Sommerfeld, Wave-Mechanics, London 1930, pp. 112 ff (English translation of Atombau und Spektrallinien. Wellenmechanischer Ergänzungsband, Braunschweig 1929), and in L. de Broglie, L'Éléctron Magnétique, Paris 1934, pp. 101 ff.

178. The Zeitschrift für Physik was generally recognised to be the organ of the 'left Wing' of German physics. After its inauguration in 1920, it soon became the most important vehicle for papers in physics, ousting the older and more conservative rival, the Annalen. Nevertheless, Schrödinger did not publish his papers on wave mechanics in the Zeitschrift, of which he, in fact, made no use after 1924. Personally and politically, Schrödinger was a conservative and a nationalist and was close to the stand of e.g. Wien. Raman and Forman

has suggested "a strange rapport between Schrödinger and the right wing of German physics," to which Wien belonged. See note 34, p. 301. This rapport did not, however, include any attack on, or doubt about Einsteinian relativity, being a favourite target for the charges of right wing physicists. Schrödinger was a firm believer in relativity.

179. Hermann (note 117) fails to recognize the improbability of this claim, based on Dirac's narrative. Hermann's 1975 biographical sketch gives a basically correct picture of Schrödinger's concern with wave mechanics; however, according to Hermann, "Schrödinger was deeply disappointed by this failure and must have thought at first that his whole method was basically wrong." (p. 219).

180. The empirical agreement of Q_1, its derivation of Bohr's formula is, of course, only apparently a result of the non-relativistic approximation. All things considered, the relativistic result was, although wrong, *better* than the non-relativistic result. However, by restricting the perspective to the non-relativistic domain, Schrödinger managed to make his readers ignore the fine-structure discrepancy, and then to present the whole matter in a convincing form.

181. Note 96.

182. "Von der relativistischen Gleichung 2-Ordnungs mit den vielen Vätern glaube ich aber nicht, dass sie der Wirklichkeit entspricht," Pauli wrote to Schrödinger 22 November 1926 (AHQP). See also note 96.

183. Most of the following account is based on the sources: O.Klein, "Ur mit liv i fysiken," Svensk Naturvetenskap, 1973, pp. 159-172 (an almost identical version may be found on pp. 59-68 in From a Life in Physics, IAEA Bulletin, 1969). I.Fischer-Hjalmars and B.Laurent, "Oskar Klein," Kosmos, 1978, pp. 19-30. C.Møller, "Oskar Klein," Fysisk Tidsskrift, 75 (1977), 169-171. AHQP interview with O.Klein, 1963.

184. Bohr and Kramers, Klein's nearest teachers and associates, greatly appreciated the talents of the largely self-learned Swede. Recommending Klein for his position in Michigan in 1923, Kramers described

Klein's work as containing a "peculiar phantasy and richness in thoughts", and that "he knows and feels physics, and all things he has published are very good, and partly of great importance." Quoted from P.Robertson, The Early Years. The Niels Bohr Institute 1921-1930, Copenhagen 1979, p. 53.

185. In his obituary of Klein, C.Møller writes: "Actually, he was, prior to Schrödinger, very close to a wave mechanical description of atomic systems in accordance with the fundamental postulates of Bohr's theory. What prevented him to be first, was presumably that he endeavoured a theory which was also in accordance with the principle of relativity, while Schrödinger at first restricted himself to consider non-relativistic atomic systems." Note 183 (my translation), p. 170. However, as is fully substantiated in this paper, relativity was not a hindrance to the creation of wave mechanics; on the contrary, such as shown by Schrödinger's relativistic theory. What maybe prevented Klein to create a wave mechanical theory, was not relativity but his attempt to go along with *general* relativity.

186. Klein (note 183, 1973), p. 163.

187. Commenting on his early ideas of a wave interpretation of quantum theory, Klein once remarked: "I had that in the back of my head when I was doing much earlier work, but I feared that it was too fantastic to be anything, so I mentioned very little about it. You know, Bohr was also very busy, so I was always afraid of distrubing him." AHQP interview of 25 February 1963. Also, im the Bohr-Klein correspondence (BSC) 1922-1925, the five-dimensional theory and wave quantum ideas are only mentioned casually.

188. "I had it [the Klein-Gordon equation] before he [Schrödinger] began the thing at all, but I hadn't published it." AHQP interview of 25 February 1963. "I had the general wave equation, I had that quite a time earlier [than Schrödinger]." AHQP interview 16 July 1963.

189. See note 222.

190. O.Klein, "Quantentheorie und fünfdimensionale Relativitätstheorie," Zs. f. Phys. 37 (1926), 895-906 (received 28 April 1926).

191. References and historical surveys of the first phases of the so-called unitary problem may be found in Whittaker (note 43), vol.2,ch.5. See also M.-A.Tonnelat, Les théories unitaires de l'électromagnétism et de la gravitation, Paris 1965, and J.Mehra, Einstein, Hilbert and the Theory of Gravitation: Historical Origins of General Relativity, Dordrecht 1975.

192. Th.Kaluza, "Zum Unitärproblem der Physik," Sitzungsber. Preuss. Akad. Wiss., 54 (1921), 966-972. Kaluza's ideas about a five-dimensional formulation appeared already in 1919 and was welcomed by Einstein. See V.V.Raman, "Theodor Kaluza," Dictionary of Scientific Biography (ed. C.C.Gillispie), vol.7, New York 1963.

193. Note 190, and O.Klein, "Zur fünfdimensionalen Darstellung der Relativitätstheorie," Zs. f. Phys., 46 (1928), 188-208.

194. H.Mandel, "Zur Herleitung die Feldgleichungen in der allgemeinen Relativitätstheorie," Zs. f. Phys., 39 (1926), 136-145.

195. A.Einstein, "Zu Kaluza's Theorie des Zusammenhanges von Gravitation und Elektrizität," Sitzungsber. Preuss. Akad. Wiss., 60 (1927), 23-25 and 26-30.

196. Note 192, and O.Klein, "The Atomicity of Electricity as a Quantum Theory Law," Nature, 118 (1926), 516 (dated 3 September 1926).

197. F.London, "Über eine Deutungsmöglichkeit der Kleinschen fünfdimensionalen Welt," Die Naturwissenschaften, 15 (1927), 15-16 (dated 17 November 1926). London's argument was to interpret m_0c^2 as a rotational spin energy with an angular momentum $d = h/2\pi$ and an 'inertial moment' θ. With $E_{rot} = m_0c^2 = d^2/\theta$ we then have $\theta = h^2(4\pi^2 m_0 c^2)^{-1}$, in virtue of which the relativistic energy equation (no field) takes the form

$$-\frac{E^2}{m_0c^2} + \frac{4\pi^2 m_0 c^2}{h^2} d^2 + \frac{\vec{p}^{\,2}}{m_0} = 0$$

By transforming to wave mechanics by means of the standard operator prescriptions (5.22) and by furthermore taking d to be the canonical conjugate to x_0, i.e., eq.(10.1), London obtained Klein's equation in free space, that is eq.(10.2) with $\varphi=0$.

198. L.Landau and D.Iwanenko, "Zur Ableitung der Klein-Fockschen Gleichung," Zeits. f. Phys., 40 (1927).

199. Note 190, p. 905.

200. O.Klein, "Elektrodynamik und Wellenmechanik von Standpunkt des Korrespondenzprinzips," Zs. f. Phys., 41 (1927), 407-442 (received 6 December 1926).

201. "I started the whole thing in relativistic mechanics because I had this five dimensional approach. I never thought that that was any important thing, just to have the relativistic scalar equation after Schrödinger's equation. But I thought that there were some other things which were important, for instance, that it was time-dependent..." AHQP interview of 25 February 1963.

202. In Leiden, Klein worked out a number of problems in wave mechanics, partly in collaboration with Uhlenbeck and Ehrenfest. Klein proposed to publish these results jointly, but Ehrenfest refused to join Klein in publishing, and the paper never got ready. The draft to this unpublished Klein-Uhlenbeck-Ehrenfest paper is deposited in the BSC. It is entitled "Einige Anwendungen der Schwingungsgleichung der Quantentheorie", and dated August 1926. It consists of various examples (Zeeman effect, dispersion and others) worked out from the non-relativistic limit of Klein's generalized version of Schrödinger's equation. For a published product of the Leiden physicists' concern with the five-dimensional theory, see P.Ehrenfest and G.E.Uhlenbeck, "Graphische Veranschaulichgung der De Broglieschen Phasenwellen in der fünfdimensionalen Welt von O.Klein," Zs. f. Phys., 39 (1926), 495-498 (received 16 September 1926).

203. L.Rosenfeld, "L'Univers à cinq dimensions et la mécanique ondulatoire," Bull. Acad. Roy. Belg., (5), 13 (1927), 304-325, 447-458, 573-579, 661-682.

204. According to a AHQP interview with Rosenfeld, 1 July 1963.

205. L. de Broglie, "L'Univers à cinq dimensions et la mécanique ondulatoire," Journal de Physique, 8 (1927), 65-73 (received 23 December 1926).

206. V.Fock, "Über die invariante Form der Wellen - und der Bewegungsgleichungen für einen geladenen Massenpunkt," Zs. f. Phys., 39 (1926), 226-232 (received 30 July 1926).

207. In one of his papers on the subject (note 193 p. 191), Klein stated in a footnote: "[Ich] halte es nicht mehr für möglich, durch die Einführung einer fünften Dimension den von der Quantentheorie geforderten Abweichungen von der Raum-Zeitbeschreibung der klassischen Theorie gerecht zu werden." In the spring of 1928, Klein has recalled (AHQP interview), he and Pauli drank a glass of wine to the death of the fifth dimension. Later on, however, Klein resumed his occupation with the five-dimensional formalism, now being applied to the Dirac equation which, if framed five-dimensionally, was thought to represent the meson field of a nucleon. See O.Klein, "Meson Fields and Nuclear Interaction," Arkiv för Mat., Astr. och Fysik, 34A, no.1, 1948, pp. 1-19.

208. Cf. V.V.Raman, "Relativity in the Early Twenties: Many-Sided Reactions to a Great Theory," Indian Journal of History of Science, 7 (1972), 119-145.

209. For references, see Jammer (note 18) and Raman, op.cit. In addition, see also E.Reichenbächer, "Welche weltgeometrischen Eigenschaften Zeichnen die gequantelten Weltlinien der Elektronen im Wasserstoffatom aus?" Zs. f. Phys., 32 (1925), 505-517. M.S.Vallarta, "Sommerfeld's Theory of Fine Structure from the Standpoint of General Relativity," J. Math. and Phys. 4 (1925), 65-83.

210. O.R.Baldwin and G.B.Jeffery, "Electronic Orbits on the Relativity Theory," Proc.Roy.Soc., A 111 (1926), 104-108.

211. Cf. notes 34 and 35.

212. Th. De Donder and Fr. van den Dungen, "La quantification déduite de la Gravifique einsteinienne," Comp. Rend., 183 (1926, 5 July), 22-24. Also: Th. de Donder, "Application de la quantification déduite de la Gravifique einsteinienne," Comp. Rend., 183 (1926, 11 October), 594-595. Th. de Donder and Fr. van den Dungen, "Sur la quantification des Systèmes relativistiques," Bull. Acad. Roy. Belg., (5), 12 (1926), 490-497.

213. H.T.Flint and J.W.Fisher, "A Contribution to Modern Ideas on the Quantum Theory," Proc. Roy. Soc., A 115 (1927), 208-215. H.T.Flint, "Relativity and the Quantum Theory," Proc. Roy. Soc., A 117 (1927), 630-637.

A.Isakson, "Zum Aufbau der Schrödingerschen Gleichung," Zs. f. Phys., 44 (1927), 893-899. F.London, "Die Theorie von Weyl und die Quantenmechanik," Die Naturwissenschaften, 15 (1927), 187; "Quantenmechanische Deutung der Theorie von Weyl," Zs. f. Phys., 42 (1927), 375-389. D.J.Struik and N.Wiener, "A Relativistic Theory of Quanta," J. Math. Phys., 7 (1927), 1-23; "The Fifth Dimension in Relativistic Quantum Theory," Proc. Nat. Acad. Sci., 14 (1928), 262-268. F.Gonseth and G.Juvet, "Les équations de l'électromagnétisme et l'equation de M. Schrödinger dans l'univers à cinq dimensions," Comp. Rend., 185 (1927), 535-538. W.Wilson, "Relativity and Wave Mechanics," Proc. Roy. Soc., A 118 (1928), 441-448.

214. In the 1958 reedition of his 1921 Handbuch article (cf. note 86), Pauli used the opportunity to include a rather detailed treatment of the five-dimensional theory of Kaluza and Klein. Pauli was then clearly sympathetic to this approach, which he saw as a possible clue to the unified field theory, still sought for. He ended his appraisal: "The question of whether Kaluza's formalism has any future in physics is thus leading to the more general unsolved main problem of accomplishing a synthesis between the general theory of relativity and quantum mechanics." (p. 232).

215. L. de Broglie, "The Beginnings of Wave Mechanics," pp. 12-25 in Wave Mechanics (note 94); p. 15.

216. L. de Broglie' "Remarques sur la nouvelle mécanique ondulatoire," Comp. Rend., 183 (19 July 1926), 272-274. Also "Les principes de la nouvelle mécanique ondulatoire," Journal de Physique, 7 (1926), 321-337.

217. Note 167.

218. Q_2, p. 513.

219. Note 131.

220. C.Eckart, "The Solution of the Problem of the Single Oscillator by a Combination of Schrödinger's Wave Mechanics and Lanczos' Field Theory," Proc. Nat. Acad. Sci., 12 (1926), 473-476.

221. Interview with O.Klein, 23 February 1963 (AHQP).

222. Letter, Pauli to Jordan, 12 April 1926. Reprinted and commented in B.L.van der Waerden, "From Matrix Mechanics and Wave Mechanics to Unified Quantum

Mechanics," pp. 276-293 in J.Mehra (ed.), The Physicist's Conception of Nature, Dordrecht 1973. A copy of Pauli's letter to Jordan was sent to Wentzel and probably also to some other physicists. See letter from Pauli to Wentzel, 8 May 1926 (AHQP).

223. Letter, Pauli to Wentzel, 5 July 1926 (AHQP). For Pauli's and others early occupation with a relativization of Schrödinger's theory, see also note 96.

224. W.Pauli and V.Weisskopf, "Über die Quantisierung der skalaren relativistischen Wellengleichung," Helv. Phys. Acta, 7 (1934), 709-731.

225. Letter, Pauli to Schrödinger, 22 November 1926 (AHQP).

226. V.Fock, "Zur Schrödingerschen Wellenmechanik," Zs. f. Phys., 38 (1926), 242-250 (received 11 June 1926).

227. C.Eckart, "The Hydrogen Spectrum in the new Quantum Theory," Phys. Rev., 28 (1926), 927-935 (dated 17 July 1926).

228. P.S.Epstein, "Two Remarks on Schrödinger's Quantum Theory," Proc. Nat. Acad. Sci., 13 (1927), 94-96.

229. F.Brouwer, "Wellenmechanische Eigenwertprobleme und Integration durch Reihen," Ann. d. Phys., 84 (1927), 915-929.

230. P.A.M.Dirac, "The Compton Effect in Wave Mechanics," Proc. Cambridge Phil. Soc., 23 (1926), 500-507 (received 8 November 1926). W.Gordon, "Der Comptoneffekt nach der Schrödingerschen Theorie," Zs. f. Phys., 40 (1927), 117-133 (received 29 September 1926). J.Kudar, "Zur vierdimensionalen Formulierung der undulatorischen Mechanik," Ann. d. Phys., 81 (1926), 632-636 (received 30 August 1926). E.Guth, "Zur Ableitung der Schrödingerschen Wellengleichung," Zs. f. Phys., 41 (1927), 235-238 (received 27 December 1926). D.Iwanenko and G.Gamow, "Zur Wellentheorie der Materie," Zs. f. Phys., 39 (1926). 865-868 (received 19 September 1926). L.Landau and D.Iwanenko, note 184. H.Bateman, "A Modification of Gordon's Equations," Phys. Rev., 30 (1927), 55-60 (received 30 March 1927).

231. See A.Haas, Materiewellen und Quantenmechanik, Leipzig 1928, pp. 36-42.

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Bernhelm Booss & Mogens Niss (eds.).

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