SOURCES OF QUANTUM MECHANICS

EDITED WITH A HISTORICAL INTRODUCTION
BY

B. L. VAN DER WAERDEN

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UNIVERSITY OF ZÜRICH



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The idea of collecting the most important early papers on Quantum Mechanics in a Source Publication is due to Max Born, and he intended to include 15 papers written by himself, Jordan, Heisenberg, Dirac and Pauli, and published during the years 1924–1926.

Dr. Paul Rosbaud, who until his death in 1963 acted as a scientific consultant to various publishing houses, took it upon him to discuss Born's project with several physicists. They all were in agreement that it would be best if all German papers were to be translated into English in order to make the sources available to all physicists and historians of Science. It was Pauli who recommended to Dr. Rosbaud the inclusion of earlier papers by Ladenburg, Kramers and Heisenberg which have prepared the way towards Quantum Mechanics.

When Dr. Rosbaud asked me to act as the editor of this volume, I discussed the list of papers with Born, Heisenberg, Heitler, Hund, Jordan, Kronig and others. They all agreed that several earlier papers written between 1917 and 1924 by Bohr, Einstein, Ehrenfest and Kuhn ought to be included, because these are necessary for a good understanding of the 'turning point' of the year 1925. At Jordan's advise, a paper by Van Vleck, which had strongly influenced Born's and Jordan's ideas on the interaction between matter and radiation, was also included in the project. However, a line had to be drawn somewhere. Therefore the following principles were adopted:

1. Papers on Quantum Theory were included only when they were judged indispensable for a proper understanding of the development of Quantum Mechanics. Thus, Bohr's great 1918 paper, in which the Principle of Correspondence was exposed, was included, but not Bohr's earlier papers. On the same principle, Planck's fundamental 1900 paper on the Law of Radiation was excluded, because a more fundamental

derivation of the same Law was given in Einstein's 1917 paper on the emission and absorption of radiation (no. 1 of the present collection). The papers of Debye and Sommerfeld, however important for the deviation of classical Quantum Theory, had to be omitted. Historia's of Science, who want to learn more about pre-1925 Quantum Theory, will have to consult Sommerfeld's 'Atombau und Spektrallinien' and Pauli's article 'Quantentheorie' in Geiger and Scheel's Handbuch der Physik, Vol. 23.

- 2. Papers on the Zeeman Effect, Spin and Statistics were left aside, because these closely related subjects have been dealt with in the Pauli Memorial Volume (Interscience Publishers 1960), p. 199–244, by B. L. van der Waerden.
- 3. Papers on Wave Mechanics were not included. We hope to assemble them in a second volume.
- 4. The papers of John von Neumann, who gave Quantum Mechanics a rigorous mathematical foundation, were also reserved for the second volume.
- 5. Papers on Quantum Field Theory are outside the scope of this collection.

Even within these limits, only the most important papers could be included. Related papers are mentioned by title at the end of each paper.

Obvious misprints in the original papers have been tacitly corrected. The papers collected in this volume naturally fall into two groups:

- (i) Towards Quantum Mechanics. Papers 1-11, by Einstein, Ehrenfest, Bohr, Ladenburg, Kramers, Slater, Born, Van Vleck, Heisenberg, and Kuhn. The German papers of this group were translated by G. Field.
- (ii) Matrix Mechanics. Papers 12-17, by Heisenberg, Born, Jordan, Dirac and Pauli. The German papers were translated by a team consisting of E. Sheldon, D. Robinson, G. Field and B. L. van der Waerden.

These two groups of papers are preceded by a historical introduction. In this introduction, use is made of letters of Heisenberg and others, which cast a new light on the history of Quantum Mechanics. Parts of these letters are reproduced in the original language.

I feel great gratitude to all who have helped me in selecting the papers and who gave me additional information. I am especially indebted to Born, Dirac, Heisenberg, Hund, Jordan, Kronig, Th. Kuhn

and Wigner, and to Mrs. Pauli, who had the great kindness of showing me letters of Heisenberg to Pauli.

Thanks are also due to the Gesellschaft der Wissenschaften in Göttingen, which has borne the considerable cost of translating the German papers into English.

B. L. van der Waerden

Zürich, September 1966

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INTRODUCTION

B. L. VAN DER WAERDEN

PART I. TOWARDS QUANTUM MECHANICS

Max Planck

Quantum theory was born on December 14, 1900, when Max Planck delivered his famous lecture before the Physikalische Gesellschaft, which was afterwards printed in Verhandlungen der Deutschen physikalischen Gesellschaft 2, p. 237 under the title 'Zur Theorie des Gesetzes der Energieverteilung im Normalspektrum'.

In this paper, Planck assumed that the emission and absorption of radiation always takes place in discrete portions of energy, or 'energy quanta' $h\nu$, where ν is the frequency of the emitted or absorbed radiation. Starting with this assumption, Planck arrived at his famous formula for the density of black-body radiation at temperature T:

$$\rho = \frac{\alpha v^3}{\exp(hv/kT) - 1}.$$

An excellent commentary to Planck's paper was given by Martin Klein in Vol. 1 of the Archive for History of Exact Sciences, p. 459 (1962). We shall not reproduce Planck's paper here, because another derivation of Planck's law, which gives a better insight into the establishment of the equilibrium between the radiation and the emitting and absorbing molecules, was given by Einstein in paper 1.

Rutherford

In order to explain the scattering of alpha particles by atoms, Rutherford assumed the atom to contain a charge +Ne or -Ne at its center surrounded by a sphere of electrification containing a charge -Ne or +Ne uniformly distributed throughout a sphere of radius R, e

being the fundamental unit of charge, and R being of the order of the radius of an atom, viz. 10^{-8} cm 1 . From these assumptions, he deduced the angular distribution of the scattered particles. The experimental results obtained by Geiger in 1910 were found to be in substantial agreement with Rutherford's theory, whereas they could not be explained by earlier theories.

The deductions from the theory are independent of the sign of the central charge, and Rutherford concludes: it has not been found possible to obtain definite evidence to determine whether it be positive or negative'. However, the drawings in the paper are made for the case of a positive central charge, and Rutherford himself seems to favour this assumption, for he writes:

If the central charge be positive, it is easily seen that a positively charged mass if released from the centre of a heavy atom, would acquire a great velocity in moving through the electric field. It may be possible in this way to account for the high velocity of expulsion of α particles without supposing that they are initially in rapid motion within the atom.

Rutherford also considers the possibility that the negative charge, instead of being uniformly distributed throughout a sphere of radius R, is located in N rotating electrons. This hypothesis was considered by Nagaoka in 1904 (Phil. Mag. 7, p. 445). Nagaoka had considered the properties of a 'Saturnian' atom, consisting of a central mass and Saturnian rings of rotating electrons. Rutherford notes that the angular distribution of scattered α -particles would be practically the same, whether the atom is considered to be a disk or a sphere, because large deviations are mainly due to the central charge.

Niels Bohr

The synthesis of Rutherford's atom model with Planck's quantum hypothesis was the great achievement of Niels Bohr. He supposed the atom to consist of a nucleus with positive charge Ze and Z electrons with charge -e each, moving according to the laws of classical mechanics. In his papers of 1913, 1914 and 1915 (Phil. Mag. 26, 27, 29 and 30) he introduced a set of assumptions concerning the stationary states of an atom and the frequency of the radiation emitted or absorbed when the atom passes from one such state to another,

- 1 E. Rutherford: The Scattering of α and β Particles by Matter and the Structure of the Atom. Phil. Mag. 21 (sixth series) p. 669. Dated April 1911.

ź

and he showed that it is possible in this way to obtain a simple interpretation of the main laws governing the line spectra of the elements, and especially to deduce the Balmer formula for the hydrogen spectrum.

We need not enter into details here, because the main principles of Bohr's theory are fully explained in Bohr's 1918 paper 3.

Bohr's ideas were further developed and applied to more complicated spectra by Sommerfeld, Debye and others. For this development we must refer the reader to Pauli's excellent article 'Quantentheorie' in Geiger-Scheel's Handbuch der Physik, 1st edition, Vol. 23 (1926), reprinted in Pauli's Collected Scientific Papers, Vol. 1. The historian should also consult Sommerfeld's Atombau und Spektrallinien (preferably 4th ed., 1924), because it was mainly from this book that the young physicists who created Quantum Mechanics in 1925–26 learnt Quantum Theory.

Einstein

In Bohr's theory, the interaction between matter and radiation remained mysterious. Why does not the atom emit radiation, when it is in its ground state? What really happens when an atom passes from one stationary state to another? What laws determine the probabilities of these transitions?

The first one to bring more light into the darkness was Einstein (paper 1). Einstein starts with Bohr's assumption that a molecule can only exist in a discrete set of states with energies ε_1 , ε_2 , If such molecules belong to a gas at temperature T, Einstein assumes, by analogy to the Boltzmann-Gibbs canonical distribution, the relative frequency W_n of a state Z_n to be 1

$$W_n = p_n \exp(-\varepsilon_n/kT)$$
,

 p_n being an integer called 'statistical weight' of the state.

In a radiation field, a molecule in state Z_n with energy ε_n may absorb radiation of frequency ν and pass to a state Z_m with higher energy ε_m . The probability for this process to happen during the time $\mathrm{d}t$ is assumed to be

$$\mathrm{d}W = B_n^m \rho \, \mathrm{d}t$$

¹ This assumption was already introduced in an earlier paper of Einstein: Verh. der D. Physik. Ges. 16, p. 820 (1914). See also Einstein's paper on Specific Heat in Annalen der Physik (4) 22, p. 180 (1907).

where ρ is the radiation density for frequency ν . Just so, a molecule in state Z_m may emit radiation and pass into a state Z_n with lower energy. The probability for this process is assumed to be

$$dW = (A_m^n + B_m^n \rho) dt.$$

If the radiation is in equilibrium with the molecular distribution of states at temperature T, the following condition must hold:

$$p_n \exp(-\epsilon_n/kT)B_n^m \rho = p_m \exp(-\epsilon_m/kT)(B_m^n \rho + A_m^n).$$

From this condition and from Wien's displacement law, Einstein derives Planck's radiation law and Bohr's frequency condition

$$\varepsilon_m - \varepsilon_n = h\nu$$
.

Einstein next assumes that in an elementary process of emission or absorption only directed radiation bundles are emitted or absorbed. He says: 'Outgoing radiation in the form of spherical waves does not exist'. For the elementary processes, he postulates the conservation of momentum and energy. The momentum of a directed radiation bundle carrying an energy hv is supposed to be hv/c, and the direction of the radiation bundle emitted from a molecule to be determined by chance. It is shown that the recoil momenta transferred from the radiation field to the molecules never disturb the thermodynamic equilibrium. This result is regarded by Einstein as a justification of his initial assumptions, for if one of these assumptions were to be changed, the result would not come out.

All subsequent research on absorption emission and dispersion of radiation was based upon Einstein's paper 1.

The Adiabatic Hypothesis

Two important heuristic principles have guided quantum physicists during the period 1913-1925, viz. Ehrenfest's Adiabatic Hypothesis and Bohr's Principle of Correspondence.

The Adiabatic Hypothesis, first formulated by Ehrenfest ¹ in 1913, says:

¹ P. Ehrenfest: Bemerkung betreffs der spezif. Wärme zweiatomiger Gase. Verh. D. physik. Ges. 15, p. 451 (1913). A Theorem of Boltzmann and its connection with the theory of quanta. Proc. Kon. Akad. Amsterdam 16, p. 591 (1913).

'If a system be affected in a reversible adiabatic way, allowed motions are transformed into allowed motions.'

The name Adiabatic Hypothesis is due to Einstein, as Ehrenfest states in paper 2. Bohr calls the hypothesis 'Principle of mechanical transformability' (see 3, § 1).

In paper 2, Ehrenfest explains what he means by a 'reversible adiabatic affection', and he formulates the Adiabatic Hypothesis as sharply as possible, at the same time showing what is wanting in sharpness. He next demonstrates the importance of adiabatic invariants, and he indicates the difficulties that arise in the application of the hypothesis in singular cases. Finally, Ehrenfest shows that the adiabatic hypothesis is closely connected with the Second Law of Thermodynamics.

The Principle of Correspondence

Bohr's fundamental 1918 paper 'The quantum theory of line spectra' consists of three parts; the fourth part announced in the introduction never appeared. Part I 'On the general theory' will be reproduced here as paper 3. Part II deals with the hydrogen spectrum. Part III, which was not published until 1922, contains a preliminary discussion of the spectra of other elements.

In Part I, Bohr once more enunciates the two fundamental assumptions of Quantum Theory:

- I. That an atomic system can only exist permanently in a discontinuous series of 'stationary states',
- II. That the radiation absorbed or emitted during a transition between two stationary states possesses a frequency ν given by

$$(1) E' - E'' = h\nu.$$

Since these assumptions imply that no emission of radiation takes place in the stationary states, it follows that the ordinary laws of electrodynamics cannot be applied to these states without radical alterations. In many cases, however, the effect of that part of the electrodynamical forces which is connected with the emission of radiation will at any moment be very small as compared with the Coulomb forces. Therefore Bohr assumes that a close approximation of the motion in the stationary states can be obtained by retaining only the Coulomb forces and calculating the motions of the particles by ordinary mechanics.

Next, Bohr considers a transition between two stationary states. He remarks that in the limiting region of slow vibrations, it has been possible to account for the phenomenon of temperature radiation by ordinary electrodynamics. Hence 'we may expect that any theory capable of describing this phenomenon in accordance with observation will form some sort of natural generalisation of the ordinary theory of radiation.'

If we analyse this argument, we see that it consists of two parts. First, Bohr expresses an experience from earlier investigations concerning the limiting region of slow vibrations, and next an expectation for future research. At this stage of Bohr's exposition, his expectation is formulated only in a qualitative form: the future theory of radiation must be a 'natural generalisation' of the classical theory.

Next, Bohr considers another limiting case, viz. the case of high quantum numbers. Once more, the starting point is a conclusion drawn from earlier research:

'We shall show ... that the conditions which will be used to determine the values of the energy in the stationary states are of such a type that the frequencies calculated by (1), in the limit where the motions in successive stationary states differ very little from each other, will tend to coincide with the frequencies to be expected on the ordinary theory of radiation from the motion of the system in the stationary states' (§ 1 of Bohr's paper 3).

Immediately after this conclusion from research already carried out, Bohr formulates an expectation for future research. He first reminds us of his earlier conclusion from the limiting case of slow vibrations:

'In order to obtain the necessary relation to the ordinary theory of radiation in the limit of slow vibrations we are therefore led directly to certain conclusions about the probability of transition between two stationary states in this limit.'

These rather vague words in § 1 are a preliminary announcement of a much more definite expectation or claim, which Bohr formulates in § 2 for the case of one degree of freedom and again in § 3 for several degrees of freedom, and which he himself later called *Principle of Correspondence*. For the moment we note two things. At first, Bohr had only said 'we may expect ...'. Now, he uses the expression 'necessary relation', which is much stronger, and he repeats it in § 2.

Secondly, we may note that Bohr, in his preliminary announcement of 'certain conclusions' in § 1, speaks about the probability of transition 'in this limit', i.e. in the limit of slow vibrations. In his more definite

statement of the Principle of Correspondence in § 2 and § 3, he considers another limiting case, viz. the case of large quantum numbers. This is not just the same thing. In many cases the two limits $n\to\infty$ and $v\to0$ coincide, but in the case of the harmonic oscillator the frequency ν remains constant while n goes to infinity. It seems that Bohr, in his preliminary announcement in § 1, did not clearly distinguish between the two limiting cases.

In § 2, after having expanded the displacements of the particles in Fourier series (14) with coefficients C_{τ} , Bohr notes that, as far as the frequencies are concerned, there exists a close relation between the ordinary theory of radiation and the new theory for large quantum numbers n. Bohr now proceeds:

In order to obtain the necessary connection, mentioned in the former section, to the ordinary theory of radiation in the limit of slow vibrations, we must further claim that a relation, as that just proved for the frequencies, will, in the limit of large n, hold also for the intensities of the different lines in the spectrum.

In this very remarkable sentence, Bohr formulates not only an expectation, but even a necessity, a claim which the future theory has to fulfill, and he concludes:

'Since now on ordinary electrodynamics the intensities of the radiations ... are directly determined from the coefficients C_{τ} in (14), we must therefore expect that for large values of n these coefficients will on the quantum theory determine the probability of spontaneous transition from a given stationary state for which n=n' to a neighbouring state for $n=n''=n'-\tau$.'

This expectation or necessary connection between the classical and the future theory in the limit of large quantum numbers, is called the *Principle of Correspondence*. The name 'Korrespondenzprinzip' is found for the first time in a later paper of Bohr: Z. Phys. 2, p. 423 (1920).

Three years later, in Z. Phys. 13 (1923), Bohr discussed anew the fundamental principles of Quantum Theory in connection with the Principle of Correspondence (paper 3h, to be quoted at the end of paper 3).

History of the Correspondence Principle

The first enunciation of an assumption akin to the Principle of Correspondence can be found already in Bohr's first paper in Phil. Mag. 26,

p. 1 (1913). Bohr speaks of the constant in the expression

$$\nu = \frac{2\pi^2 m e^4}{h^3} \left(\frac{1}{\tau_2^2} - \frac{1}{\tau_1^2} \right) \tag{4}$$

- the number (4) is Bohr's - and he proceeds:

From the above consideration it will follow that, taking the starting point in the form of the law of the hydrogen spectrum and assuming that the different lines correspond to a homogeneous radiation emitted during the passage between different stationary states, we shall arrive at exactly the same expression for the constant as that given in (4), if we only assume 1) that the radiation is sent out in quanta hv, and 2) that the frequency of the radiation emitted during the passing of the system between successive stationary states will coincide with the frequency of revolution of the electron in the region of slow vibrations.

For a fuller discussion of the development and meaning of the Principle of Correspondence in Bohr's papers we may refer to K. M. Meyer-Abich: Korrespondenz, Individualität und Komplementarität, Dissertation Hamburg 1964.

Applications of the Correspondence Principle

In § 2 of his fundamental paper 3, Bohr applies the Principle of Correspondence to the special case in which certain coefficients C_{τ} are zero. In this case

we are led to expect that no transition will be possible for which n'-n'' is equal to one of these values τ .

Quite similar is Bohr's conclusion in the case of several degrees of freedom (see the end of Bohr's paper).

A successful application of this point of view to the intensity and polarization of the Stark components in hydrogen-like spectra was given by Kramers in his papers of 1919 and 1920, to be quoted at the end of Bohr's paper 3.

Systematic guessing

The research work during the years 1919-1925 that finally led to Quantum Mechanics may be described as systematic guessing, guided by the Principle of Correspondence.

An important step in this direction was made in 1921 by Ladenburg in paper 4. Kramers, in his papers 6 and 8, improved on Ladenburg's results. The three papers 4, 6 and 8 are not easy to understand for a