Jagdish Mehra Helmut Rechenberg

The Historical Development of Quantum Theory

VOLUME 5

Erwin Schrödinger and the Rise of Wave Mechanics

Part 1

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Dedicated to the Memory of Erwin Schrödinger (12 August 1887-4 January 1961) on the Centenary of His Birth

Abbreviated Contents—Part 2

The Creation of Wave Mechanics; Early Response and Applications 1925–1926

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Foreword

The date of 12 August 1987 marks the hundredth anniversary of Erwin Schrödinger's birth. Schrödinger's name is linked with an equation which is, by far, the most-often quoted in the scientific literature of the twentieth century. The Schrödinger equation occurs regularly in papers not only by physicists working in a variety of fields—from atomic and molecular physics to solid state, nuclear and elementary particle physics—but nearly as often in papers on topics of theoretical chemistry—both organic and inorganic—and occasionally even in biological papers. Even more justly than Einstein's popular mass-energy relation, $E = mc^2$, the Schrödinger equation should be taken as the most characteristic equation of twentieth-century science.

The Schrödinger equation is more than just a mathematical relation. It denotes a complete mathematical and physical method of describing atoms, molecules and submicroscopic particles, appropriately called undulatory mechanics or wave mechanics. This theory explicitly involves previously unknown aspects of matter, especially in the domain of atomic and subatomic phenomena. Historically, the establishment of wave mechanics—the initial steps towards it, as well as its final formulation—can be linked almost exclusively with the name of Erwin Schrödinger, though a few important contributions to it were also made by a small number of other physicists. Being a very complex, highly cultivated and erudite person, Schrödinger took a rather sophisticated path to his atomic theory, which emerged rather late in his professional career. Therefore, without a review of the scientific work and ideas of the young Schrödinger, his publications on wave mechanics in early 1926 must appear an unbelievable wonder. The reconstruction of the origins of wave mechanics demands a detailed and careful analysis of Schrödinger's development as a person and as a scientist, one whose interests extended far beyond the borders of physics and science in general. Consideration of everything that Schrödinger did-experimental and theoretical physics, statistical physics and meteorology, colour theory and physiological optics, biology and philosophy, as well as poetry—becomes inevitable, because all these things were somehow intimately interwoven in his mind.

In order to present the extensive material pertaining to the makeup of Schrödinger's personality and his scientific development, we have divided the present volume into two parts, each containing two chapters. Part 1, entitled 'Schrödinger in Vienna and Zurich 1887-1925', deals with the prehistory of wave mechanics. In Chapter I, on 'Schrödinger in Vienna 1887-1920', we discuss Schrödinger's Viennese background, his youth and studies at the University of Vienna, his early

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scientific work (on kinetic theory, atmospheric electricity, the atomic structure of solids and other topics), his duties as an artillery officer during World War I, and scientific work during the war years (on statistical physics, general relativity, atomic and quantum theory), and his concern with philosophy. In Chapter II, on 'Waves and Quanta: Preludes to Wave Mechanics', we concentrate, after summarizing the recognition of the dual nature of light and reviewing the side-stages of the development of quantum theory, mainly on the scientific development of Erwin Schrödinger in the 1920s. We discuss his arrival in Zurich, Switzerland, and the main ideas that he brought to his new environment. At first, during the early years in Zurich, quantum theory and the analysis of atomic structure did not lie at the centre of Schrödinger's scientific interests-though he did consider selected problems of atomic structure, besides his work on the radiation problem and physiological optics at that time. Statistical mechanics was a far more important occupation and a continuous field of research for Schrödinger. He had been interested in this subject from his student days in Vienna, and now in Zurich he published, from 1922 to 1926, a series of papers on it. These investigations on statistical mechanics must be viewed as contributing a crucial step, apart from Louis de Broglie's conception of matter waves, to the genesis of wave mechanics.

Part 2, entitled 'The Creation of Wave Mechanics; Early Response and Applications 1925-1926', is again divided into two chapters (III and IV). In Chapter III, on 'The Creation of Wave Mechanics', we make an attempt to recreate the steps that, in our view, led to the actual rise of wave mechanics in the hands of Schrödinger: the scientific exchange with Planck and Einstein on the fundamental questions of statistical mechanics, his initial steps towards a relativistic hydrogen equation, his correspondence with Wilhelm Wien and the development of the nonrelativistic hydrogen equation, the fundamental conceptual sources of undulatory mechanics, the foundation of undulatory mechanics, and the initial reception of the new theory by Wilhelm Wien and Arnold Sommerfeld. In Chapter IV, on 'Early Response and Applications', we discuss Schrödinger's early extension of the wave equation to atomic problems, the continuation of correspondence with Wien and Sommerfeld, the response to wave mechanics from Planck, Einstein and Lorentz, the establishment of the formal equivalence of Schrödinger's wave mechanics and the quantum mechanics of Born, Heisenberg, Jordan and Dirac, by Schrödinger himself and by Pauli and Carl Eckart. We also discuss the early applications and generalization of the wave mechanical scheme by Erwin Fues (diatomic molecules), Ivar Waller, Gregor Wentzel, Carl Eckart and Paul Epstein (Stark effect and the hydrogen spectrum), Max Born (collision processes in wave mechanics), Werner Heisenberg (the helium problem) and Paul Dirac (symmetry properties of wave functions and quantum statistics). Further, we discuss the initial steps towards the interpretation of the new atomic mechanics taken by Schrödinger (and the reactions of certain physicists to it), including his visits to Berlin and Munich to present his theory, his discussions there with Planck, Einstein, Wien and Sommerfeld, and to Copenhagen for his Foreword

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discussions with Niels Bohr. We close the last section with further fundamental applications and developments of wave mechanics in the second half of 1926 (such as the contributions of Schrödinger himself, Charles Manneback, Fritz Reiche, Walter Gordon, Gregor Wentzel, Oskar Klein, Vladimir Fock, Janos Kudar, Théophile De Donder, Frans van den Dungen, J. Robert Oppenheimer, Waldemar Alexandrow, Øyvind Burrau, Ralph Kronig, Isidor Rabi and others), which served to increase the fame of its creator who would soon succeed Max Planck in the chair of theoretical physics in Berlin.

For the purpose of our account of the prehistory, the birth and rise of wave mechanics, we have first made use of the primary sources: Schrödinger's published papers, his unpublished notebooks and memoranda, as well as his scientific correspondence (with Pauli, Sommerfeld, Wien, Planck, Einstein, Lorentz, and others); we have also made use of interviews and discussions with, and the recollections of, many physicists, including Born, Dirac, Heisenberg, Eckart, Debye, Fues, Uhlenbeck, and others, and we have benefited from other secondary sources including historical articles, dissertations and accounts of the reminiscences concerning Schrödinger's life and scientific work.

We wish to thank Professors Ilya Prigogine, Abdus Salam, Willis E. Lamb, Jr. and Eugene P. Wigner for their continuous encouragement during the writing of this work.

We take great pleasure in presenting this result of our efforts to readers in the scientific community.

25 December 1986

Jagdish Mehra Helmut Rechenberg

Acknowledgments

Erwin Schrödinger's scientific papers have been reprinted recently in Erwin Schrödinger: Gesammelte Abhandlungen, Volumes 1-4 (Vienna, 1984). Many of his essays and selections from other writings have been collected together and published as books. Selected letters exchanged by Schrödinger with Max Planck, Albert Einstein and Hendrik Antoon Lorentz were edited in Briefe zur Wellenmechanik (1963) and in an English translation, as Letters on Wave Mechanics (1967). Copies of large parts of his unpublished diaries, manuscripts, notebooks and notes on physical, philosophical and other topics, as well as his scientific correspondence and an interview with his widow, Frau Annemarie Schrödinger, have been filed on microfilms deposited in the Archives for the History of Quantum Physics at the American Philosophical Society, Philadelphia, Pa. We are deeply indebted to Schrödinger's daughter, Frau Ruth Braunizer, Alpbach (Tyrol), Austria, for her generous permission to quote from Schrödinger's correspondence and his published and unpublished writings.

Copies of Erwin Schrödinger's scientific correspondence with Albert Einstein are contained in the duplicate of the Einstein Archives, Sealy G. Mudd Library, Princeton, N.J. We are grateful to Charles E. Bloom and Ehud Benamy of the American Friends of the Hebrew University, Inc., New York, N.Y., for handling the arrangements to obtain permission to quote from Einstein's writings and correspondence; these materials are published by permission of the Hebrew University of Jerusalem, Israel.

Schrödinger's correspondence with Arnold Sommerfeld and Wilhelm Wien is contained in the Sommerfeld and Wien Collections at the *Deutches Museum*, Munich, Federal Republic of Germany. We are grateful to the *Deutches Museum* for permission to quote from this correspondence.

We are indebted to the Stiftung Preußischer Kulturbesit. Berlin, Federal Republic of Germany, for making available the Schrödinger Landé correspondence contained in the Alfred Landé Collection.

The scientific correspondence of Wolfgang Pauli up to 1.39 has been published in Wolfgang Pauli: Wissenschaftlicher Briefwechsel/Scientific Correspondence, Volume I (1979) and Volume II (1985). For permission to quote from Pauli's correspondence, we are indebted to Frau Franca Pauli, Victor F. Weisskopf and Springer-Verlag.

For permission to make use of the resources of the Niels Bohr Archives in Copenhagen, Denmark, and to quote from them, we are grateful to Aage Bohr.

We have drawn upon the reminiscences and the conversations and discussions of one of us (J.M.) with several quantum physicists (including Max Born, P. A. M. Dirac and Werner Heisenberg). We have also made use of the interviews of the Sources for the History of Quantum Physics with Max Born, Peter Debye, Paul Dirac, Carl Eckart, Erwin Fues, Werner Heisenberg, George E. Uhlenbeck, and others. For help in making use of the materials contained in the Archives for the History of Quantum Physics, we are grateful to the Manuscript Librarian, American Philosophical Society, Philadelphia, Pa.

Ample literature dealing with Erwin Schrödinger and wave mechanics exists, especially when compared with that on the matrix branch of quantum mechanics. In addition to articles in various scientific books and journals, several doctoral dissertations have also been devoted to the subject. Of the latter, we mention two: Linda A. Wessels' Schrödinger's Interpretations of Wave Mechanics (Indiana University, 1975), and Paul A. Hanle's Erwin Schrödinger's Statistical Mechanics (Yale University, 1975). William T. Scott's book, Erwin Schrödinger: An Introduction to His Writings (Amherst, Mass., 1967), contains Schrödinger's bibliography and an introductory essay on his life and on his scientific and popular writings. We have benefited from these accounts.

We are grateful to the Instituts Internationaux de Physique et de Chimie (Solvay), Université Libre de Bruxelles, Brussels, Belgium, and Alfried Krupp von Bohlen und Halbach-Stiftung, Essen-Bredeney, Federal Republic of Germany, for grants in aid of the publication of this volume.

JAGDISH MEHRA
HELMUT RECHENBERG

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General Introduction

In issue No. 4 of Annalen der Physik, whose editing was completed on 13 March 1926, there appeared a paper written by Erwin Schrödinger in Zurich bearing the title 'Quantisierung als Eigenwertproblem. (Erste Mitteilung)' ('Quantization as a Problem of Eigenvalues. Part I', Schrödinger, 1926c). Four weeks later, Wolfgang Pauli from Hamburg wrote in a letter to Pascual Jordan in Göttingen:

Today I want to write neither about my Handbook-Article [on quantum theory, which occupied Pauli at that time: Pauli, 1926b] nor about multiple quanta [in radiation theory, which occupied Jordan then]; I will rather tell you the results of some considerations of mine connected with Schrödinger's paper "Quantisierung als Eigenwertproblem" which just appeared in the Annalen der Physik. I feel that this paper is to be counted among the most important recent publications. Please read it carefully and with devotion. (Pauli to Jordan, 12 April 1926; English translation of the German text in Van der Waerden, 1973, p. 278)

In the following months Schrödinger published five further papers extending his method to what he called wave mechanics and applied it to a variety of problems in atomic theory (Schrödinger, 1926d, e, f, g, h). Many years later, Max Born said in an obituary of Schrödinger: 'What is more magnificent in theoretical physics than his first six papers on wave mechanics?' ('Was gibt es Großartigeres in der theoretischen Physik als seine ersten sechs Arbeiten zur Wellenmechanik?': Born, 1961a, p. 85).

Born, as well as Jordan and Pauli belonged among the pioneers who had developed, since the middle of 1925, a new version of atomic theory which they called 'quantum mechanics'. This development had emerged in a more or less direct way from the quantum theory of atomic structure, introduced by Niels Bohr in 1913 and extended afterwards by him and Arnold Sommerfeld to describe a large number of atomic systems.

From the Bohr-Sommerfeld Theory to Quantum Mechanics

The original scheme of Bohr and Sommerfeld represented a mixture of classical dynamics and quantum requirements or conditions, the latter determining the stationary states of atoms and molecules. However, the spectra emitted by those objects did not obey the laws of classical electrodynamics, where the electron is supposed to move around the atomic nuclei due to classical dynamics. The frequencies emitted and absorbed were given rather by the (classical) energy

differences between the stationary states, or more accurately by those energy differences divided by Planck's quantum-theoretical constant h. Thus the ingenious mixture of classical theory and quantum-theoretical ideas, which was applied for over a decade—i.e., from 1913 to 1925—with ever-increasing skill and endurance to more and more complex atomic systems, did not rest on a consistent theoretical basis. Especially, the electrodynamics of James Clerk Maxwell—a theory which accounted so well for all phenomena of static and stationary electromagnetic phenomena and for electromagnetic waves and their propagation, reflection and diffraction—lost its validity when applied to the processes of creation and absorption of radiation in atoms.

Still one was able to reach a fair agreement between experimental and theoretical results in many examples, if one just stuck to the set of inconsistent rules implied in the Bohr-Sommerfeld theory of atomic structure. However, since 1922 a deeper analysis of the properties possessed by atoms with several electrons, or even by one-electron atoms under peculiar external conditions, had revealed increased failures of the theory. A more adequate quantum-theoretical description of the scattering of light by atoms, properly named the 'dispersion-theoretic approach'—as inaugurated in 1924 by Niels Bohr and his collaborators in Copenhagen and Max Born and his associates in Göttingen-however, fostered some distant hopes of gradually resolving all the fundamental discrepancies existing between experiment and theory. The theory, or, more accurately, the rules of this dispersion-theoretic scheme demanded: (i) replacing certain differential expressions in the classical description of atoms and their interaction with radiation by difference expressions, and (ii) substituting in the latter, for any (classical) frequency, the observed (quantum) frequency of radiation. From the dispersion-theoretic scheme, which the members of the Bohr school called occasionally 'the sharpened correspondence principle', there emerged in little more than a year the first consistent atomic theory.

The pioneering paper, in which the basic principles of the new theory were formulated, stemmed from Werner Heisenberg in Göttingen, a former student of Sommerfeld, Born and Bohr. In July 1925 he expounded emphatically that the main deficiency of the old, unsuccessful atomic theory (of Bohr and Sommerfeld) lay in the use of several concepts that did not correspond to observable quantities, these quantities, such as the orbital motion of electrons in atoms and molecules, should therefore be forbidden in future, and Heisenberg demanded that only observable quantities should occur in a consistent theory (Heisenberg, 1925c). In practice, he described periodic atomic systems by 'quantum-theoretical Fourier series,' whose amplitudes were the transition amplitudes between stationary states and whose frequencies were the corresponding atomic frequencies. These quantum-theoretical Fourier series represented the dynamical variables in the new theory; they obeyed equations of motion, whose structure resembled the corresponding equations in classical dynamics. A remarkable difference with the classical theory, however, showed up in the fact that products of two quantumtheoretical variables or Fourier series did not necessarily commute. Heisenberg further presented in his paper the solution of the simplest quantum systems, i.e.,

of the anharmonic oscillator and the rigid rotator, believing them capable of describing essentially the observed features of real atoms.

The Göttingen Matrix Mechanics and Its Extensions

Heisenberg's colleagues in Göttingen, Born and Jordan, then obtained in the summer of 1925 a suitable mathematical scheme formulating the physical ideas of Heisenberg's 'quantum-theoretical reformulation' of the old atomic theory. They rewrote, in particular, the quantum-theoretical Fourier series as infinite Hermitean matrices and established within a matrix theory a description of atomic systems analogous to the Hamilton-Jacobi theory of classical systems (Born and Jordan, 1925b). The matrix mechanics provided a direct mathematical representation of the discreteness involved in the quantum concept.

Matrix mechanics allowed one to treat, in principle, any multiply-periodic system of atomic theory, provided one succeeded in finding suitable dynamical variables that could be described by Hermitean matrices (Born, Heisenberg and Jordan, 1926). As a special example, Wolfgang Pauli solved in October 1925 the hydrogen problem in matrix mechanics, i.e., he calculated the energy states of the hydrogen atom and reproduced Bohr's old result of 1913 in agreement with observation; at the same time he overcame a difficulty that had bothered the old atomic theory, because the matrix mechanical solution of the crossed-field problem did not lead to inconsistencies (Pauli, 1926a).

A little later than Born and Jordan, in the fall of 1925, Paul Adrien Maurice Dirac in Cambridge, also starting from Heisenberg's July paper, provided an even more general quantum-mechanical scheme than matrix mechanics (Dirac, 1925d). His theory, in which he represented the quantum-theoretical variables by what he called 'q-numbers,' allowed one to take over the classical Hamiltonian theory more directly than was possible in matrix mechanics, thus offering the opportunity to deal with any kind of many-electron atoms and even with the relativistic problem of Compton scattering (Dirac, 1926a, b, c).

The new quantum mechanics, whether expressed in the matrix formulation of Born and Jordan or in the q-number formulation of Dirac, showed one characteristic feature: in its equations, say, the equations of motion, differences of products of dynamical variables appeared instead of differential expressions of classical mechanics. The very nature of the new quantum theory seemed therefore to rest, so the people in Göttingen, Copenhagen and Cambridge claimed, in the algebraic structure of its equations. However, in December 1925, Max Born and Norbert Wiener, who collaborated at the Massachusetts Institute of Technology, submitted a paper showing that the gap between the classical and the quantum mechanical treatment was not really so large as reflected in matrix or q-number theory: in their method of 'operator mechanics' not only the differential equation form of classical dynamics recurred; in certain cases, such as the uniform motion of a particle in a straight line, the quantum-theoretical problem also had the same solution as the corresponding classical problem (Born and Wiener, 1926a, b).

A similar consequence was derived even more explicitly in the 'field-like' formulation, which Cornelius Lanczos in Frankfurt proposed also in December 1925 (Lanczos, 1926a). He used explicitly the mathematical result already discovered twenty years earlier by David Hilbert in Göttingen, namely, the mathematical equivalence of the problem of solving integral equations of the Fredholm type on the one hand, and of obtaining the eigenvalues of an infinite matrix on the other hand (Hilbert, 1904a, b; 1905; 1906a, b; 1910). Lanczos reversed Hilbert's original procedure leading from the continuum problem (connected with integral equations) to the discrete problem (connected with matrices); thus he simply rewrote the matrix equations of Born and Jordan as linear integral equations. This rewriting implied the advantage, 'that all results of the theory [i.e., of quantum mechanics]... thus obtain a formulation which may appear to the physicist, who is used to working with analytical methods, more natural than the matrix formulation' (Lanczos, 1926a, p. 812). Lanczos also said: 'As far as the interpretation of the facts, that is, the real nature of the quanta, is concerned, however, one cannot exclude that the integral [equation] formulation is even superior to the matrix formulation; the reason is that it has the advantage of being immediately consistent with the field conception, indeed is even built on it, while the field concept is obviously far removed from the discontinuum formulation' (Lanczos, 1926a, pp. 812-813).

Status of Quantum Mechanics in Early 1926

The discoveries and results of Heisenberg, Born, Jordan, Dirac, Pauli, Wiener and Lanczos, determined the picture of quantum mechanics during most of the first half of 1926. The theory seemed to be successful in describing the behaviour of atomic and molecular systems, especially their discrete energy states; in a very special example, namely that of the uniform motion of a particle in a straight line—as treated by Born and Wiener—it also showed itself to be capable of accounting for a continuous energy spectrum. Hence it possessed all the prerequisites of a scheme that could describe the phenomena in atomic physics completely.

Of course, the detailed application of quantum mechanics in one of the four equivalent formulations—that of Born, Heisenberg and Jordan (matrix mechanics), of Dirac (q-number theory), of Born and Wiener (operator mechanics), or Lanczos (integral equation representation)—to practical problems other than the most elementary ones already treated (i.e., the anharmonic oscillator, the rigid rotator, the hydrogen atom, and the motion of a particle in a straight line) had still to be shown; but promising progress was obtained, e.g., in treating the problem of diatomic molecules (Mensing, 1926a). Both in Europe and the United States (where, in particular, Born had imported quantum mechanics) many physicists were eagerly looking for problems that could be attacked within the new theory. One generally hoped to be able to cope with all problems of atomic theory in this way, provided one just tried hard enough and invented clever tricks, such as Pauli had employed in the case of the nonrelativistic