

# QUANTUM MECHANICS

BY

LEONARD I. SCHIFF

*Professor of Physics  
Stanford University*

FIRST EDITION

**交通書店**

上海(20)徐家匯華山路1988號

電話：七八五二三

1949

## PREFACE

This volume has a threefold purpose: to explain the physical concepts of quantum mechanics, to describe the mathematical formalism, and to present illustrative examples of both the ideas and the methods. The book is intended to serve as a text at the graduate level and also as a reference book. It is assumed that the reader is reasonably familiar with atomic structure, classical mechanics, and differential equations: In addition, he should have had some contact with electromagnetic theory and, for the latter part of the book, with the special theory of relativity.

The author believes that the analytical methods employed in the book will satisfy most theoretical physicists even though no attempt is made to achieve mathematical rigor. For example, there is little or no discussion of the justification for the interchange of sum, derivative, and integral operations, or for the use of the  $\delta$  function. On the other hand, the physical reasons for the nature of the results obtained are investigated wherever possible.

Problems are given at the end of each chapter. They are often used to illustrate or amplify points discussed in the text. Original theoretical papers are referred to throughout the book; the list is representative rather than exhaustive. Experimental results are, for the most part, quoted without reference, since the large amount of documentation required for an adequate survey seems out of place in a book on theoretical physics. Several other books on quantum mechanics and related subjects are referred to for more detailed discussions of particular topics.

The scope of this volume is best outlined if the book is divided into three parts. The first three chapters constitute an introduction to quantum mechanics, in which the physical concepts are discussed and the Schrödinger wave formalism is established. The detailed treatment of the wave function (Chap. III) may be omitted in a first reading. The next eight chapters comprise the central part of the book. This part presents exact solutions of the wave equation for both energy-level and collision problems, the Heisenberg matrix formalism and transformation theory, approximation methods, radiation theory, and some applications to atomic systems. Since the first eleven chapters correspond to a typical one-year graduate course, it seemed desirable to include a semi-classical treatment of electromagnetic radiation in the central part of the book (Chap. X) even though some of the results are obtained again in Chap. XIV. The last part of the book corresponds to a short course in what is often called advanced quantum mechanics. It consists of rela-

tivistic particle theory and an introduction to quantized field theory and quantum electrodynamics.

Nearly all this book was written while the author was at the University of Pennsylvania, and he gratefully acknowledges the continued encouragement of Prof. G. P. Harnwell. He is also indebted to Drs. E. H. Kennard and S. Pasternack for helpful criticism of the early chapters, to W. Miller and L. Spruch for their careful reading of most of the manuscript, and to Profs. F. Bloch, R. F. Christy, and W. W. Hansen for valuable comments on certain sections. It is a particular pleasure for the author to thank Prof. R. Serber for many discussions of both the conceptual and formal aspects of quantum mechanics that took place during the last eleven years.

Finally, the author wishes to acknowledge his indebtedness to Prof. J. R. Oppenheimer for his introduction to several of the ideas and examples that appear in the book. Indeed, the writing of this book in its present form owes much to the period from 1937 to 1940, which the author spent in association with Professor Oppenheimer.

LEONARD I. SCHIFF

STANFORD, CALIFORNIA  
June, 1948

# CONTENTS

PREFACE . . . . .	v
-------------------	---

## CHAPTER I

### THE PHYSICAL BASIS OF QUANTUM MECHANICS

1. <i>Experimental Background</i> . . . . .	1
Inadequacy of classical physics. Summary of principal experiments and inferences.	
2. <i>The Old Quantum Theory</i> . . . . .	3
Bohr-Sommerfeld quantization rules. Practical difficulties. Conceptual difficulties. Quantum-mechanical viewpoint.	
3. <i>Uncertainty and Complementarity</i> . . . . .	6
Uncertainty principle. Complementarity principle. Limitations on experiment.	
4. <i>Discussion of Measurement</i> . . . . .	9
Analysis of diffraction experiment. Discussion of diffraction experiment. Localization experiment.	
5. <i>Wave Packets in Space and Time</i> . . . . .	12
Space packets. Time packets. Wave formalism.	

## CHAPTER II

### THE SCHRÖDINGER WAVE EQUATION

6. <i>Development of the Wave Equation</i> . . . . .	17
Traveling harmonic waves. Need for a wave equation. The one-dimensional wave equation. Extension to three dimensions. Inclusion of forces.	
7. <i>Interpretation of the Wave Function</i> . . . . .	21
Statistical interpretation. Normalization of $\psi$ . Probability current density. Expectation value. Ehrenfest's theorem.	
8. <i>Energy Eigenfunctions</i> . . . . .	27
Separation of the wave equation. Significance of the separation constant $E$ . Boundary conditions at great distances. Continuity conditions. Boundary conditions for infinite potential energy. Energy eigenvalues in one dimension. Discrete energy levels. Continuous energy eigenvalues. Discrete and continuous eigenvalues in three dimensions.	
9. <i>One-Dimensional Square Well Potential</i> . . . . .	34
Perfectly rigid walls. Finite potential step. Energy levels. Parity. A simplified solution.	

## CHAPTER III

### EIGENFUNCTIONS AND EIGENVALUES

10. <i>Interpretative Postulates and Energy Eigenfunctions</i> . . . . .	41
Dynamical variables as operators. Expansion in eigenfunctions. The	

	total energy operator. Normalization in a box. Orthonormality of energy eigenfunctions. Reality of the energy eigenvalues. Expansion in energy eigenfunctions. The closure property. Probability function and expectation value. General solution of the Schrödinger equation.	
11.	<i>Momentum Eigenfunctions</i> . . . . .	48
	Form of the eigenfunctions. Box normalization. The Dirac $\delta$ function. A representation of the $\delta$ function. Normalization in terms of the $\delta$ function. Some properties of the $\delta$ function. Closure. Expansion in momentum eigenfunctions. Probability function and expectation value.	
12.	<i>Motion of a Free Wave Packet in One Dimension</i> . . . . .	54
	The minimum uncertainty product. Form of the minimum packet. Momentum expansion coefficients. Change with time of a minimum packet. Classical limit.	

## CHAPTER IV

## DISCRETE EIGENVALUES: ENERGY LEVELS

13.	<i>Linear Harmonic Oscillator</i> . . . . .	60
	Asymptotic behavior. Energy levels. Zero-point energy. Parity. Hermite polynomials. Harmonic-oscillator wave functions. Correspondence with classical theory. Oscillating wave packet.	
14.	<i>Spherically Symmetric Potentials in Three Dimensions</i> . . . . .	69
	Separation of the wave equation. Legendre polynomials. Spherical harmonics. Parity. Angular momentum.	
15.	<i>Three-Dimensional Square Well Potential</i> . . . . .	76
	Zero angular momentum. Interior solutions for arbitrary $l$ . Exterior solutions for arbitrary $l$ . Energy levels.	
16.	<i>The Hydrogen Atom</i> . . . . .	80
	Reduced mass. Asymptotic behavior. Energy levels. Laguerre polynomials. Hydrogen-atom wave functions. Degeneracy. Separation in parabolic coordinates. Energy levels. Wave functions.	

## CHAPTER V

## CONTINUOUS EIGENVALUES: COLLISION THEORY

17.	<i>One-Dimensional Square Potential Barrier</i> . . . . .	92
	Asymptotic behavior. Normalization. Scattering Coefficients.	
18.	<i>Collisions in Three Dimensions</i> . . . . .	96
	Scattering cross section. Relations between angles in the laboratory and center-of-mass systems. Relation between cross sections. Dependence on $\gamma$ . Asymptotic behavior. Normalization.	
19.	<i>Scattering by Spherically Symmetric Potentials</i> . . . . .	103
	Asymptotic behavior. Scattering cross section. Phase shifts. Calculation of $\delta_l$ . Relation between signs of $\delta_l$ and $V(r)$ . Ramsauer-Townsend effect. Scattering by a perfectly rigid sphere. Scattering by a square well potential. Resonance scattering. Angular distribution at low energies.	
20.	<i>Scattering by a Coulomb Field</i> . . . . .	114
	Parabolic coordinates. Confluent hypergeometric function. Scattering cross section and normalization. Solution in spherical coordinates. Modified Coulomb field. Classical limit for a pure Coulomb field.	

## CHAPTER VI

## MATRIX FORMULATION OF QUANTUM MECHANICS

21. *Matrix Algebra* . . . . . 122  
 Matrix addition and multiplication. Null, unit, and constant matrices. Spur, determinant, and inverse of a matrix. Hermitian and unitary matrices. Transformation and diagonalization of matrices. Matrices of infinite rank.
22. *Matrices in Quantum Mechanics* . . . . . 127  
 A unitary transformation matrix. Hamiltonian matrix. Dynamical variables as Hermitian matrices. Wave functions as unitary matrices. The  $r$  representation. A useful identity.
23. *Equations of Motion in Matrix Form* . . . . . 131  
 Time rate of change of a matrix. Classical Lagrangian and Hamiltonian equations of motion. Poisson brackets and commutator brackets. Quantization of a classical system. Motion of a particle in an electromagnetic field. Evaluation of commutator brackets. Velocity and acceleration of a charged particle. The Lorentz force. Constants of the motion. The parity operator. Energy representation.
24. *Angular Momentum* . . . . . 140  
 Definition of angular momentum. Choice of a representation. Relations between matrix elements. Eigenvalues of  $M_z$ . Eigenvalues of  $M^2$ ; the  $L$ -matrix. Connection with the spherical harmonics. Spin angular momentum. Addition of angular momenta. Eigenvalues of  $(M_1 + M_2)^2$ .

## CHAPTER VII

## APPROXIMATION METHODS FOR STATIONARY PROBLEMS

25. *Stationary Perturbation Theory* . . . . . 149  
 Nondegenerate case. First-order perturbation. Second-order perturbation. Normalization of  $\psi$ . Perturbation of an oscillator. Degenerate case. Removal of degeneracy in first order. Removal of degeneracy in second order. First-order Stark effect in hydrogen. Perturbed energy levels. Occurrence of permanent electric-dipole moments.
26. *The Born Approximation* . . . . . 159  
 Perturbation approximation. Green's function. Green's function for a free particle. Explicit evaluation. Scattering cross section. Perturbation treatment of partial waves. Phase shifts. Scattering by a square well potential. Validity of the Born approximation. Scattering by a screened Coulomb field.
27. *The Variation Method* . . . . . 169  
 Expectation value of the energy. Application to excited states. Ground state of helium. Electron interaction energy. Variation of the parameter  $Z$ . van der Waals interaction. Perturbation calculation. Variation calculation.
28. *The WKB Approximation* . . . . . 178  
 Classical limit. Approximate solutions. Asymptotic nature of the solutions. Solution near a turning point. Linear turning point. Connection at the turning point. Asymptotic connection formulas. Energy levels of a potential well. A quantization rule. Special boundary conditions.

## CHAPTER VIII

## APPROXIMATION METHODS FOR TIME-DEPENDENT PROBLEMS

29. *Time-Dependent Perturbation Theory* . . . . . 189  
 Expansion in unperturbed eigenfunctions. First-order perturbation. Physical interpretation. Transition probability. Scattering cross section. Harmonic perturbation. Second-order perturbation. Effect of first-order transitions. Intermediate states.
30. *Inelastic Collisions* . . . . . 199  
 Expression for the cross section. Evaluation of the matrix element. Differential and total cross sections. Production of a cloud-chamber track. Formulation of the problem. Evaluation of the  $k$  sum. Second-order matrix element. Discussion of the cross section.
31. *Adiabatic and Sudden Approximations* . . . . . 207  
 Expansion in instantaneous energy eigenfunctions. Choice of phases. Adiabatic approximation. Connection with perturbation theory. Discontinuous change in  $H$ . Sudden approximation. Transient disturbance. Disturbance of an oscillator.

## CHAPTER IX

## IDENTICAL PARTICLES AND SPIN

32. *Identical Particles* . . . . . 216  
 Physical meaning of identity. Symmetric and antisymmetric wave functions. Construction from unsymmetrized functions. Distinguishability of identical particles. The exclusion principle. Connection with statistical mechanics. Collisions of identical particles.
33. *Spin Angular Momentum* . . . . . 223  
 Connection between spin and statistics. Spin matrices and eigenfunctions. Collisions of identical particles. Electron spin functions. The helium atom. Spin functions for three electrons.
34. *Rearrangement Collisions* . . . . . 230  
 Notation for rearrangement collisions. Use of the Born approximation. Lack of orthogonality of initial and final states. Connection with time-dependent perturbation theory. Exchange collisions of electrons with hydrogen. Differential cross section. Exchange collisions with helium.

## CHAPTER X

## SEMICLASSICAL TREATMENT OF RADIATION

35. *Absorption and Induced Emission* . . . . . 240  
 Maxwell's equations. Plane electromagnetic waves. Use of perturbation theory. Transition probability. Interpretation in terms of absorption and emission. Electric-dipole transitions. Forbidden transitions.
36. *Spontaneous Emission* . . . . . 248  
 Classical radiation field. Asymptotic form. Radiated energy. Dipole radiation. Angular momentum. Dipole case. Conversion from classical to quantum theory. Planck distribution formula. Line breadth.
37. *Some Applications of Radiation Theory* . . . . . 257  
 Selection rules for a single particle. Polarization of emitted radiation.

Conservation of angular momentum. Selection rules for many-particle systems. Cerenkov effect. Expression for the current density. Fourier analysis of the radiation field. Radiated energy.

## CHAPTER XI

## ATOMS, MOLECULES, AND ATOMIC NUCLEI

38. *Approximations in Atomic Structure* . . . . . 267  
 Central-field approximation. Periodic system of the elements. Thomas-Fermi statistical model. Evaluation of the potential. Hartree's self-consistent fields. Connection with the variation method. Corrections to the central-field approximation. *LS* coupling scheme. Selection rules. *jj* coupling scheme.
39. *The Alkali Atoms* . . . . . 279  
 Doublet separation. Doublet intensity. Effect of a magnetic field. Weak-field case. Strong-field case. Quadratic Zeeman effect.
40. *Molecules* . . . . . 288  
 Classification of energy levels. Wave equation. The hydrogen molecule. Potential-energy function. The Morse potential. Rotation and vibration of diatomic molecules. Energy levels. Effect of nuclear identity.
41. *Atomic Nuclei*. . . . . 297  
 General properties of nuclei. Nature of nuclear interactions. Nuclear models. Neutron-proton system. Exchange operators. Proton-proton scattering.

## CHAPTER XII

## RELATIVISTIC WAVE EQUATIONS

42. *Schrödinger's Relativistic Equation* . . . . . 306  
 Free particle. Electromagnetic potentials. Separation of the equation. Energy levels in a Coulomb field.
43. *Dirac's Relativistic Equation*. . . . . 311  
 Free-particle equation. Matrices for  $\alpha$  and  $\beta$ . Free-particle solutions. Charge and current densities. Electromagnetic potentials.
44. *Dirac's Equation for a Central Field* . . . . . 319  
 Spin angular momentum. Approximate reduction; spin-orbit energy. Separation of the equation. The hydrogen atom. Classification of energy levels. Negative energy states.

## CHAPTER XIII

## THE QUANTIZATION OF WAVE FIELDS

45. *Classical and Quantum Field Equations*. . . . . 329  
 Coordinates of the field. Lagrangian equation. Functional derivative. Hamiltonian equations. Quantum equations for the field. Fields with more than one component.
46. *Quantization of the Nonrelativistic Schrödinger Equation*. . . . . 336  
 Lagrangian and Hamiltonian equations. Quantum equations. The  $N$  representation. Connection with the harmonic oscillator. Physical interpretation. Connection with the many-particle Schrödinger equation.



- Anticommutation relations. Equation of motion. Physical implications of anticommutation. Representation of the anticommuting  $a_k$  operators.
47. *Quantization of the Dirac Equation*. . . . . 348  
 Lagrangian and Hamiltonian equations. Quantum equations. The  $N$  representation. Negative energy states and positrons. Anticommutation relations at different times. Commutation relation for the charge density.

## CHAPTER XIV

## QUANTUM ELECTRODYNAMICS

48. *Electromagnetic Field in Vacuum*. . . . . 361  
 Lagrangian equations. Hamiltonian equations. Quantum equations. Commutation relations for  $\mathbf{E}$  and  $\mathbf{H}$ . Plane wave representation. Quantized field energy. Quantized field momentum.  $\mathbf{A}(\mathbf{r}, t)$  in the plane wave representation. Commutation relations at different times.
49. *Interaction Between Electrons and the Electromagnetic Field*. . . . . 373  
 Lagrangian and Hamiltonian equations. Elimination of  $\phi$ . Quantization of the fields. Inclusion of static fields. Use of perturbation theory. Matrix elements of the Coulomb interaction.
50. *Radiation Theory*. . . . . 382  
 Formulation in terms of transition probabilities. Matrix elements of the perturbation. Transition probability for absorption. Transition probability for emission. Analysis of a diffraction experiment. Representation of the electromagnetic field. Matrix elements. Classical diffraction pattern.
- INDEX. . . . . 397

## CHAPTER I

### THE PHYSICAL BASIS OF QUANTUM MECHANICS

At the present stage of human knowledge, quantum mechanics can be regarded as the fundamental theory of atomic phenomena. The experimental data on which it is based are derived from physical events that lie almost entirely beyond the range of direct human perception. It is not surprising, therefore, that the theory embodies physical concepts that are foreign to common daily experience. These concepts did not appear in the historical development of quantum mechanics, however, until a quite complete mathematical formalism had been evolved. The need for quantitative comparison with observation, which is the ultimate test of any physical theory, in this case led first to the formalism and only later to its interpretation in physical terms.

It seems desirable in introducing the subject of quantum mechanics to depart from the historical order and preface the mathematical development with a discussion of the physical concepts. In this chapter we first review briefly the experimental background and the ideas of the old quantum theory, then discuss the newer physical concepts of uncertainty and complementarity, and finally lay the groundwork for the formalism that will be developed in its most familiar form in Chap. II. No attempt will be made to deduce the structure of the formalism from the fundamental experiments; we shall try to make the theoretical development seem plausible rather than unique. The justification for the theory, then, will rest on the agreement between deductions made from it and experiments, and on the simplicity (in principle more than in practice) and consistency of the formalism.

#### 1. EXPERIMENTAL BACKGROUND

Experimental physics prior to 1900 had demonstrated the existence of a wide variety of phenomena, which for the most part were believed to be explicable in terms of what we now call *classical* theoretical physics. The motions of mechanical objects were successfully discussed in terms of Newton's equations on both celestial and terrestrial scales. Application of this theory to molecular motions produced useful results in the kinetic theory of gases, and the discovery of the electron by J. J. Thomson in 1897 consisted in showing that it behaved like a Newtonian particle.

The wave nature of light had been strongly suggested by the diffraction experiments of Young in 1803, and was put on a firmer foundation by Maxwell's discovery in 1864 of the connection between optical and electrical phenomena.

**Inadequacy of Classical Physics.** The difficulties in the understanding of experimental results that remained at the beginning of this century were largely concerned with the development of a suitable atomic model and with the late discoveries of X rays and radioactivity. However, there were also difficulties associated with phenomena that should have been understood but actually were not: such things as the spectral distribution of thermal radiation from a black body, the low-temperature specific heats of solids, and the appearance of only 5 degrees of freedom in the motion of a free diatomic molecule at ordinary temperatures.

The beginning of an understanding of the second class of difficulties was made by Planck in 1900, when he was able to explain the black-body spectrum in terms of the assumed emission and absorption of electromagnetic radiation in discrete *quanta*, each of which contains an amount of energy  $E$  that is equal to the frequency of the radiation  $\nu$  multiplied by a universal constant  $h$  (called *Planck's constant*):

$$E = h\nu \quad (1.1)$$

This quantum idea was later used by Einstein in accounting for some of the experimental observations on the photoelectric effect. In this way the dual character of electromagnetic radiation became established: it sometimes behaves like a wave motion, and sometimes like a stream of corpuscular quanta.

At about this time, the existence of discrete values for the measurable parameters of atomic systems (not only of electromagnetic radiation) became apparent through Einstein's and Debye's theories of the specific heats of solids, Ritz's classification of spectral lines, the experiment of Franck and Hertz on the discrete energy losses of electrons on collision with atoms, and (somewhat later) the experiment of Stern and Gerlach, which showed that the component of the magnetic moment of an atom along an external magnetic field has discrete values.

**Summary of Principal Experiments and Inferences.** The theoretical physics of the first quarter of this century thus contained two important inferences, obtained from the experiments and their interpretations, that had not existed in 1900: the dual character of electromagnetic radiation, and the existence of discrete values for physical quantities. The relations between the principal experimental conclusions and the theoretical inferences are shown schematically in Table 1; for a more detailed dis-

discussion and a bibliography, reference should be made to a book on atomic physics.<sup>1</sup>

TABLE 1. RELATIONS BETWEEN EXPERIMENTAL INTERPRETATIONS AND THEORETICAL INFERENCE

Diffraction (Young 1803, Laue 1912).....	}	Electromagnetic waves
Black-body radiation (Planck 1900)		}
Photoelectric effect (Einstein 1904)	}	
Compton effect (1923)		}
Combination principle (Ritz-Rydberg 1908)	}	
Specific heats (Einstein 1907, Debye 1912)		}
Franck-Hertz experiment (1913)	}	
Stern-Gerlach experiment (1922)		}

A third theoretical inference appeared in 1924 with the suggestion by de Broglie that matter also has a dual (particle-like and wave-like) character; he assumed that the relation between the momentum  $p$  of the particle and the length  $\lambda$  of the corresponding wave is<sup>2</sup>

$$\lambda = \frac{h}{p} \tag{1.2}$$

Up to that time all the evidence had indicated that matter was composed of discrete Newtonian particles; in particular, sharp tracks of charged particles such as electrons and helium nuclei had been observed in expansion cloud chambers like that invented by C. T. R. Wilson in 1911. Shortly after this, however, Davisson and Germer (1927) and G. P. Thomson (1928) independently observed the diffraction of electrons by crystals, and thus confirmed de Broglie's principal supposition.

## 2. THE OLD QUANTUM THEORY

What is now called the *old quantum theory*<sup>3</sup> was initiated by the work of Planck on black-body radiation, and carried farther by Einstein and Debye. However, it was only after Rutherford's discovery in 1911 that an atom consists of a small, massive, positively charged nucleus surrounded by electrons, that the theory could be applied to a quantitative description of atoms.

<sup>1</sup> See, for example, F. K. Richtmyer and E. H. Kennard, "Introduction to Modern Physics" (McGraw-Hill, New York, 1942); M. Born, "Atomic Physics" (Blackie, Glasgow, 1946).

<sup>2</sup> Equation (1.2) is also valid for light quanta, as may be seen by dividing both sides of Eq. (1.1) by the velocity of light  $c$ ; for a directed beam of light  $p = E/c$  and  $\lambda = c/\nu$ .

<sup>3</sup> For a more detailed discussion than is presented in this section, see the books cited above, and L. Pauling and E. B. Wilson, Jr., "Introduction to Quantum Mechanics," Chap. II (McGraw-Hill, New York, 1935).

**Bohr-Sommerfeld Quantization Rules.** The first step in this direction was taken by Bohr in 1913, when he made two postulates concerning the electronic or extranuclear structure of an atom. The first of these was that an atomic system can exist in particular stationary or quantized states, each of which corresponds to a definite energy of the system. Transitions from one stationary state to another are accompanied by the gain or loss, as the case may be, of an amount of energy equal to the energy difference between the two states; the energy gained or lost appears as a quantum of electromagnetic radiation, or as internal or kinetic energy of another system. The second postulate (in agreement with that of Planck and Einstein) was that a radiation quantum has a frequency equal to its energy divided by Planck's constant  $h$ .

These two postulates by themselves provided some insight into the Ritz combination principle and the Franck-Hertz experiment. To obtain specific results for hydrogen, Bohr proposed a simple rule for the selection of those circular orbits which are to constitute stationary states: the angular momentum must be an integral multiple of  $h/2\pi$ . A more general quantization rule was discovered independently by W. Wilson (1915) and by Sommerfeld (1916), thus making possible the application of Bohr's postulates to a wider variety of atomic systems. This rule is applicable to Hamiltonian systems in which the coordinates are cyclic variables, and states that the integral of each canonical momentum with respect to its coordinate over a cycle of its motion must be an integral multiple of  $h$ . The rule was applied with considerable success to the computation of the fine structure of hydrogen, the spectra of diatomic molecules, and other problems.

**Practical Difficulties.** The old quantum theory encountered practical difficulties in several different respects. It could not be applied to aperiodic systems, it provided only a qualitative and incomplete treatment of the intensities of spectral lines, and it did not give a satisfactory account of the dispersion of light. Moreover, improvements in experimental techniques soon showed that there were problems, such as the rotational spectra of some diatomic molecules, to which the theory gave unambiguous but incorrect answers.

The correspondence principle was introduced by Bohr in 1923 in an effort to make use of the classical theory as a limiting case to infer some properties of atomic systems, especially the intensities of spectral lines. Although much was achieved in this way, it was clear in the early 1920's that the quantum theory as it then existed was unsatisfactory.

**Conceptual Difficulties.** Quite apart from the practical difficulties outlined above, the old quantum theory failed to give a conceptually satisfactory account of the fundamental phenomena. It was difficult to

understand why the electrostatic interaction between a hydrogen nucleus and an electron should be effective when the ability of the accelerated electron to emit electromagnetic radiation disappeared in a stationary state. The mechanism of emission and absorption of radiation in transitions between stationary states was obscure. The quantization rules were arbitrary even when they were most effective. And the assumption of a dual character for light (particle-like on emission and absorption and wave-like in transit) seemed to be self-contradictory.

In order to illustrate the conceptual difficulties and the way in which they are dealt with by the new quantum mechanics, we consider in some detail a simple diffraction experiment, which is illustrated schematically in Fig. 1. A light source  $S$  illuminates a diaphragm  $A$  in which two slits

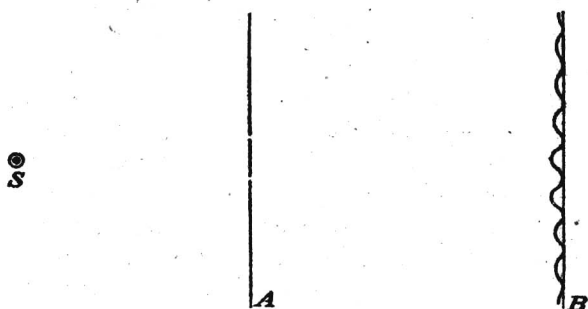


FIG. 1. A diffraction experiment in which light from  $S$  passes through the two slits in  $A$  to form a diffraction pattern at  $B$ .

are cut. A diffraction pattern appears at a photosensitive screen  $B$ , and the ejected photoelectrons are most numerous at the diffraction peaks. Here we have the radiation behaving as a wave during its passage from source through slits to screen, but behaving as a stream of light quanta or photons when it ejects electrons from  $B$ . We now know that a similar experiment could be set up with matter instead of radiation. The diffraction pattern of electrons scattered from a crystal (analogous to the slits in  $A$ ) may be detected as a distribution of electron tracks in a Wilson cloud chamber (analogous to the screen  $B$ ), so that the wave and particle aspects of matter appear in the same experiment.

In the situation illustrated in Fig. 1, we might at first suppose that the diffraction pattern is due to an interference between different photons passing through the two slits, thus explaining the observations entirely in terms of the particle picture. That this is not a sufficient explanation may be shown by decreasing the intensity of the light until an average of only one photon at a time is in transit between source and screen. The diffraction pattern still appears as the distribution of the large number of photons accumulated over a sufficiently long time. Thus we must con-

clude that diffraction is a statistical property of a single photon, and does not involve an interaction between photons. From the point of view of the particle picture, we may then ask how it is that a stream of independent photons, each of which presumably can go through only one of the slits, can produce a diffraction pattern that appears only when both slits are open. Or to put the question in another way, how can the presence of a slit through which a photon does not go prevent that photon from reaching a part of the screen it would be likely to reach if that slit were closed?

**Quantum-mechanical Viewpoint.** In this question is implicit the assumption that the photon actually does go through a particular one of the two slits. This assumption is natural from the point of view of the classical theory or the old quantum theory since these theories regard a photon or other particle as having a definite and determinable position at each instant of time. The quantum mechanics, however, discards this assumption, and asserts instead that the position of a photon has meaning only when the experiment includes a position determination. Moreover, this part of the experiment will affect the remainder of the experiment and cannot be considered separately. Thus from the point of view of quantum mechanics, the question asked in the last paragraph is without meaning, since it assumes that the photon goes through a particular one of the two slits (thus making it possible to close the other slit) when there is no provision in the experiment for determining through which slit the photon actually goes.

The quantum mechanics resolves the situation by telling us that the diffraction pattern is destroyed if a sufficiently careful attempt is made to determine through which slit each photon passes. (see Sec. 4). We must then be prepared to forego the customary mental picture of a photon (or an electron) as a classical particle that has at each instant of time a position that can be determined without damage to diffraction patterns of the type discussed here. Thus classical causality, which requires that the motion of a particle at any time be uniquely determinable from its motion at an earlier time, must also be abandoned. The new theory that is forced upon us in this way is so successful in other respects as well that, at the present state of knowledge, we must regard such classically incomplete descriptions as a fundamental property of nature.

### 3. UNCERTAINTY AND COMPLEMENTARITY

Before presenting a more quantitative discussion of the diffraction experiment outlined in Sec. 2, we consider two principles that express in qualitative terms the physical content of the theory of quantum

mechanics. We restrict ourselves here to a discussion of their meaning, and give arguments for their validity in Sec. 4.

**Uncertainty Principle.** The first of these is the *uncertainty principle*, developed by Heisenberg<sup>1</sup> in 1927. According to this principle, it is impossible to specify precisely and simultaneously the values of both members of particular pairs of physical variables that describe the behavior of an atomic system. The members of these pairs of variables are canonically conjugate to each other in the Hamiltonian sense: a rectangular coordinate  $x$  of a particle and the corresponding component of momentum  $p_x$ , a component  $J_z$  of angular momentum of a particle and its angular position  $\phi$  in the perpendicular ( $xy$ ) plane, the energy  $E$  of a particle and the time  $t$  at which it is measured, etc. Put more quantitatively, the uncertainty principle states that the order of magnitude of the product of the uncertainties in the knowledge of the two variables must be at least Planck's constant  $h$  divided by  $2\pi$  ( $\hbar \equiv h/2\pi = 1.054 \times 10^{-27}$  erg-second),<sup>2</sup> so that

$$\Delta x \cdot \Delta p_x \gtrsim \hbar \tag{3.1}$$

$$\Delta \phi \cdot \Delta J_z \gtrsim \hbar \tag{3.2}$$

$$\Delta t \cdot \Delta E \gtrsim \hbar \tag{3.3}$$

The relation (3.1) means that a component of the momentum of a particle cannot be precisely specified without our loss of all knowledge of the corresponding component of its position at that time, that a particle cannot be precisely localized in a particular direction without our loss of all knowledge of its momentum component in that direction, and that in intermediate cases the product of the uncertainties of the simultaneously measurable values of corresponding position and momentum components is at least of the order of magnitude of  $\hbar$ . Similarly, Eq. (3.2) means, for example, that the precise measurement of the angular position of a particle in an orbit carries with it the loss at that time of all knowledge of the component of angular momentum perpendicular to the plane of the orbit. Equation (3.3) means that an energy determination that has an accuracy  $\Delta E$  must occupy at least a time interval  $\Delta t \sim \hbar/\Delta E$ ; thus if a system maintains a particular state of motion not longer than a time  $\Delta t$ , the energy of the system in that state is uncertain by at least the amount  $\Delta E \sim \hbar/\Delta t$ , since  $\Delta t$  is the longest time interval available for the energy determination. The smallness of  $h$  makes the uncertainty principle of interest primarily in connection with systems of atomic size.

<sup>1</sup> W. Heisenberg, *Zeits. f. Physik*, **43**, 172 (1927).

<sup>2</sup> R. T. Birge, *Rev. Mod. Phys.* **13**, 233 (1941).



As we shall see in Sec. 12, the uncertainty principle may be obtained directly from the mathematical formulation of the theory, and this is actually the way in which it was first obtained by Heisenberg.

**Complementarity Principle.** In order to understand the implications of the uncertainty principle in more physical terms, Bohr<sup>1</sup> introduced the *complementarity principle* in 1928. This principle states that atomic phenomena cannot be described with the completeness demanded by classical dynamics; some of the elements that complement each other to make up a complete classical description are actually mutually exclusive, and these complementary elements are all necessary for the description of various aspects of the phenomena. From the point of view of the experimenter, the complementarity principle asserts that the physical apparatus available to him has such properties that more precise measurements than those indicated by the uncertainty principle cannot be made.

This is not to be regarded as a deficiency of the experimenter or of his techniques. It is rather a law of nature that, whenever an attempt is made to measure precisely one of the pair of canonical variables, the other is changed by an amount that cannot be too closely calculated without interfering with the primary attempt. This is fundamentally different from the classical situation, in which a measurement also disturbs the system that is under observation, but the amount of the disturbance can be calculated and taken into account. Thus the complementarity principle typifies the fundamental limitations on the classical concept that the behavior of atomic systems can be described independently of the means by which they are observed.

**Limitations on Experiment.** In the atomic field, we must choose between various experimental arrangements, each designed to measure the two members of a pair of canonical variables with different degrees of precision that are compatible with the uncertainty relations. In particular, there are two extreme arrangements, each of which measures one member of the pair with great precision. According to classical theory, these extreme experimental arrangements complement each other; the results of both may be obtained at once and are necessary to supply a complete classical description of the system. In quantum mechanics, however, the extreme complementary experiments are mutually exclusive and cannot be performed together.

It is in this sense that the classical concept of causality disappears in the atomic field. There is causality in so far as the quantum laws that describe the behavior of atoms are perfectly definite; there is not, however, a causal relationship between successive configurations of an

<sup>1</sup> N. Bohr, *Nature*, **121**, 580 (1928); "Atomic Theory and the Description of Nature," especially Part II (Cambridge, London, 1934); *Phys. Rev.*, **48**, 696 (1935).