# 1

# THE DISCOVERY OF QUANTUM MECHANICS

## I. INTRODUCTION

The laws of classical mechanics were summarized in 1686 by *Isaac Newton* (1642–1727) in his famous book *Philosophiae Naturalis Principia Mathematica*. During the following 200 years, they were universally used for the theoretical interpretation of all known phenomena in physics and astronomy. However, towards the end of the nineteenth century, new discoveries related to the electronic structure of atoms and molecules and to the nature of light could no longer be interpreted by means of the classical Newtonian laws of mechanics. It therefore became necessary to develop a new and different type of mechanics in order to explain these newly discovered phenomena. This new branch of theoretical physics became known as quantum mechanics or wave mechanics.

Initially quantum mechanics was studied solely by theoretical physicists or chemists, and the writers of textbooks assumed that their readers had a thorough knowledge of physics and mathematics. In recent times the applications of quantum mechanics have expanded dramatically. We feel that there is an increasing number of students who would like to learn the general concepts and fundamental features of quantum mechanics without having to invest an excessive amount of time and effort. The present book is intended for this audience.

We plan to explain quantum mechanics from a historical perspective rather than by means of the more common axiomatic approach. Most fundamental concepts of quantum mechanics are far from self-evident, and they gained general

**TABLE 1-1. Pioneers of Quantum Mechanics**

Niels Henrik David Bohr (1885–1962)
Max Born (1882–1970)
Louis Victor Pierre Raymond, Duc de Broglie (1892–1989)
Pieter Josephus Wilhelmus Debije (1884–1966)
Paul Adrien Maurice Dirac (1902–1984)
Paul Ehrenfest (1880–1933)
Albert Einstein (1879–1955)
Samuel Abraham Goudsmit (1902–1978)
Werner Karl Heisenberg (1901–1976)
David Hilbert (1862–1943)
Hendrik Anton Kramers (1894–1952)
Wolfgang Ernst Pauli (1900–1958)
Max Karl Ernst Ludwig Planck (1858–1947)
Erwin Rudolf Josef Alexander Schrödinger (1887–1961)
Arnold Johannes Wilhelm Sommerfeld (1868–1951)
George Eugene Uhlenbeck (1900–1988)

acceptance only because there were no reasonable alternatives for the interpretation of new experimental discoveries. We believe therefore that they may be easier to understand by learning the motivation and the line of reasoning that led to their discovery.

The discovery of quantum mechanics makes an interesting story, and it has been the subject of a number of historical studies. It extended over a period of about 30 years, from 1900 to about 1930. The historians have even defined a specific date, namely, December 14, 1900, as the birth date of quantum mechanics. On that date the concept of quantization was formulated for the first time.

The scientists who made significant contributions to the development of quantum mechanics are listed in Table 1.1. We have included one mathematician in our list, namely, David Hilbert, a mathematics professor at Göttingen University in Germany, who is often regarded as the greatest mathematician of his time. Some of the mathematical techniques that were essential for the development of quantum mechanics belonged to relatively obscure mathematical disciplines that were known only to a small group of pure mathematicians. Hilbert had studied and contributed to these branches of mathematics, and he included the material in his lectures. He was always available for personal advice with regard to mathematical problems, and some of the important advances in quantum mechanics were the direct result of discussions with Hilbert. Eventually his lectures were recorded, edited, and published in book form by one of his assistants, *Richard Courant* (1888–1972). The book, *Methods of Mathematical Physics*, by R. Courant and D. Hilbert, was published in 1924, and by a happy coincidence it contained most of the mathematics that was important for the study and understanding of quantum mechanics. The book became an essential aid for most physicists.

Richard Courant was a famous mathematician in his own right. He became a colleague of Hilbert's as a professor of mathematics in Göttingen, and he was instrumental in establishing the mathematical institute there. In spite of his accomplishments, he was one of the first Jewish professors in Germany to be dismissed from his position when the Nazi regime came to power (together with Max Born, who was a physics professor in Göttingen). In some respects Courant was fortunate to be one of the first to lose his job because at that time it was still possible to leave Germany. He moved to New York City and joined the faculty of New York University, where he founded a second institute of mathematics. Born was also able to leave Germany, and he found a position at Edinburgh University.

It may be of interest to mention some of the interpersonal relations between the physicists listed in Table 1-1. Born was Hilbert's first assistant and Sommerfeld was Klein's mathematics assistant in Göttingen. After Born was appointed a professor in Göttingen, his first assistants were Pauli and Heisenberg. Debije was Sommerfeld's assistant in Aachen and when the latter became a physics professor in Munich, Debije moved with him to Munich. Kramers was Bohr's first assistant in Copenhagen, and he succeeded Ehrenfest as a physics professor in Leiden. Uhlenbeck and Goudsmit were Ehrenfest's students. We can see that the physicists lived in a small world, and that they all knew each other.

In this chapter, we present the major concepts of quantum mechanics by giving a brief description of the historical developments leading to their discovery. In order to explain the differences between quantum mechanics and classical physics, we outline some relevant aspects of the latter in Chapter 3. Some mathematical topics that are useful for understanding the subject are presented in Chapter 2. In subsequent chapters, we treat various simple applications of quantum mechanics that are of general interest. We attempt to present the material in the simplest possible way, but quantum mechanics involves a fair number of mathematical derivations. Therefore, by necessity, some mathematics is included in this book.

## II. PLANCK AND QUANTIZATION

The introduction of the revolutionary new concept of quantization was a consequence of Planck's efforts to interpret experimental results related to black body radiation. This phenomenon involves the interaction between heat and light, and it attracted a great deal of attention in the latter part of the nineteenth century.

We have all experienced the warming effect of bright sunlight, especially when we wear dark clothing. The sunlight is absorbed by our dark clothes, and its energy is converted to heat. The opposite effect may be observed when we turn on the heating element of an electric heater or a kitchen stove. When the heating element becomes hot it begins to emit light, changing from red to white. Here the electric energy is first converted to heat, which in turn is partially converted to light.
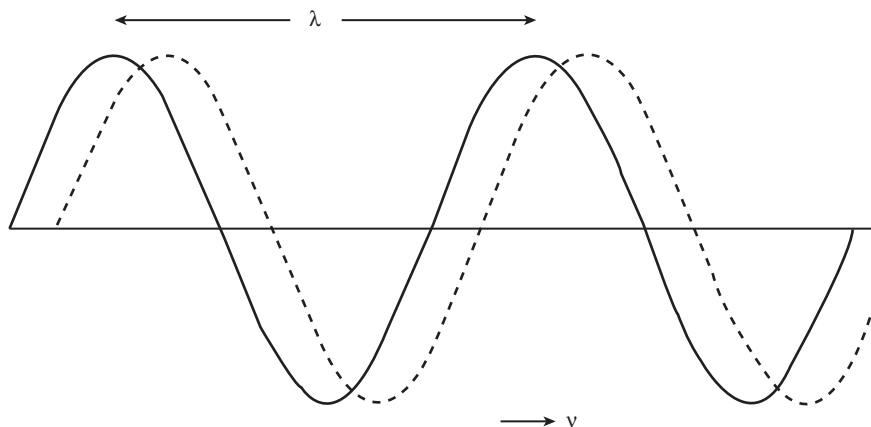
**Figure 1-1**   Sketch of a one-dimensional wave.

It was found that the system that was best suited for quantitative studies of the interaction between light and heat was a closed container since all the light within the vessel was in equilibrium with its walls. The light within such a closed system was referred to as black body radiation. It was, of course, necessary to punch a small hole in one of the walls of the container in order to study the characteristics of the black body radiation. One interesting finding of these studies was that these characteristics are not dependent on the nature of the walls of the vessel.

We will explain in Chapter 4 that light is a wavelike phenomenon. A wave is described by three parameters: its propagation velocity $\upsilon$; its wavelength $\lambda$, which measures the distance between successive peaks; and its frequency $\nu$ (see Figure 1-1). The frequency is defined as the inverse of the period $T$, that is, the time it takes the wave to travel a distance $\lambda$. We have thus

$$\upsilon = \lambda/T = \lambda\nu \tag{1-1}$$

White light is a composite of light of many colors, but monochromatic light consists of light of only one color. The color of light is determined solely by its frequency, and monochromatic light is therefore light with a specific characteristic frequency $\nu$. All different types of light waves have the same propagation velocity $c$, and the frequency $\nu$ and wavelength $\lambda$ of a monochromatic light wave are therefore related as

$$c = \lambda\nu \tag{1-2}$$

It follows that a monochromatic light wave has both a specific frequency $\nu$ and a specific wavelength $\lambda$.

The experimentalists were interested in measuring the energy of black body radiation as a function of the frequency of its components and of temperature. As more experimental data became available, attempts were made to represent these data by empirical formulas. This led to an interesting controversy because it turned out that one formula, proposed by *Wilhelm Wien* (1864–1928), gave an accurate representation of the high-frequency data, while another formula, first proposed by *John William Strutt, Lord Rayleigh* (1842–1919), gave an equally good representation of the low-frequency results. Unfortunately, these two formulas were quite different, and it was not clear how they could be reconciled with each other.

Towards the end of the nineteenth century, a number of theoreticians attempted to find an analytic expression that would describe black body radiation over the entire frequency range. The problem was solved by Max Planck, who was a professor of theoretical physics at the University of Berlin at the time. Planck used thermodynamics to derive a formula that coincided with Wien's expression for high frequencies and with Rayleigh's expression for low frequencies. He presented his result on October 19, 1900, in a communication to the German Physical Society. It became eventually known as Planck's radiation law.

Even though Planck had obtained the correct theoretical expression for the temperature and frequency dependence of black body radiation, he was not satisfied. He realized that his derivation depended on a thermodynamic interpolation formula that, in his own words, was nothing but a lucky guess.

Planck decided to approach the problem from an entirely different direction, namely, by using a statistical mechanics approach. Statistical mechanics was a branch of theoretical physics that described the behavior of systems containing large numbers of particles and that had been developed by *Ludwig Boltzmann* (1844–1906) using classical mechanics.

In applying Boltzmann's statistical methods, Planck introduced the assumption that the energy $E$ of light with frequency $\nu$ must consist of an integral number of energy elements $\varepsilon$. The energy $E$ was therefore quantized, which means that it could change only in a discontinuous manner by an amount $\varepsilon$ that constituted the smallest possible energy element occurring in nature. We are reminded here of atomic theory, in which the atom is the smallest possible amount of matter. By comparison, the energy quantum is the smallest possible amount of energy. We may also remind the reader that the concept of quantization is not uncommon in everyday life. At a typical auction the bidding is quantized since the bids may increase only by discrete amounts. Even the Internal Revenue Service makes use of the concept of quantization since our taxes must be paid in integral numbers of dollars, the financial quanta.

Planck's energy elements became known as quanta, and Planck even managed to assign a quantitative value to them. In order to analyze the experimental data of black body radiation, Planck had previously introduced a new fundamental constant to which he assigned a value of $6.55 \times 10^{-27}$ erg sec. This constant is now known as Planck's constant and is universally denoted by the symbol $h$. Planck proposed that the magnitude of his energy elements or quanta was given by

$$\varepsilon = h\nu \qquad (1\text{-}3)$$

Many years later, in 1926, the American chemist *Gilbert Newton Lewis* (1875–1946) introduced the now common term photon to describe the light quanta.

Planck reported his analysis at the meeting of the German Physical Society on December 14, 1900, where he read a paper entitled ''On the Theory of the Energy Distribution Law in the 'Normalspectrum.''' This is the date that historians often refer to as the birth date of quantum mechanics.

Privately Planck believed that he had made a discovery comparable in importance to Newton's discovery of the laws of classical mechanics. His assessment was correct, but during the following years his work was largely ignored by his peers and by the general public.

We can think of a number of reasons for this initial lack of recognition. The first and obvious reason was that Planck's paper was hard to understand because it contained a sophisticated mathematical treatment of an abstruse physical phenomenon. A second reason was that his analysis was not entirely consistent even though the inconsistencies were not obvious. However, the most serious problem was that Planck was still too accustomed to classical physics to extend the quantization concept to its logical destination, namely, the radiation itself. Instead Planck introduced a number of electric oscillators on the walls of the vessel, and he assumed that these oscillators were responsible for generating the light within the container. He then applied quantization to the oscillators or, at a later stage, to the energy transfer between the oscillators and the radiation. This model added unnecessary complications to his analysis.

Einstein was aware of the inconsistencies of Planck's theory, but he also recognized the importance of its key feature, the concept of quantization. In 1905 he proposed that this concept should be extended to the radiation field itself. According to Einstein, the energy of a beam of light was the sum of its light quanta $h\nu$. In the case of monochromatic light, these light quanta or photons all have the same frequency and energy, but in the more general case of white light they may have different frequencies and a range of energy values.

Einstein used these ideas to propose a theoretical explanation of the photoelectric effect. Two prominent physicists, *Joseph John Thomson* (1856–1940) and *Philipp Lenard* (1862–1947), discovered independently in 1899 that electrons could be ejected from a metal surface by irradiating the surface with light. They found that the photoelectric effect was observed only if the frequency of the incident light was above a certain threshold value $\nu_0$. When that condition is met, the velocity of the ejected electrons depends on the frequency of the incident light but not on its intensity, while the number of ejected electrons depends on the intensity of the light but not on its frequency.

Einstein offered a simple explanation of the photoelectric effect based on the assumption that the incident light consisted of the light quanta $h\nu$. Let us further suppose that the energy required to eject one electron is defined as $eW$, where $e$ is the electron charge. It follows that only photons with energy in excess of $eW$ are capable of ejecting electrons; consequently

$$h\nu_0 = eW \tag{1-4}$$

A photon with a frequency larger than $\nu_0$ has sufficient energy to eject an electron and, its energy surplus $E$

$$E = h\nu - eW \tag{1-5}$$

is equal to the kinetic energy of the electron. The number of ejected electrons is, of course, determined by the number of light quanta with frequencies in excess of $\nu_0$. In this way, all features of the photoelectric effect were explained by Einstein in a simple and straightforward manner. Einstein's theory was confirmed by a number of careful experiments during the following decade. It is interesting to note that the threshold frequency $\nu_0$ corresponds to ultraviolet light for most metals but to visible light for the alkali metals (e.g., green for sodium). The excellent agreement between Einstein's equation and the experimental data gave strong support to the validity of the quantization concept as applied to the radiation field.

The idea became even more firmly established when it was extended to other areas of physics. The specific heat of solids was described by the rule of Dulong and Petit, which states that the molar specific heats of all solids have the same temperature-independent value. This rule was in excellent agreement with experimental bindings as long as the measurements could not be extended much below room temperature. At the turn of the twentieth century, new techniques were developed for the liquefaction of gases that led to the production of liquid air and, subsequently, liquid hydrogen and helium. As a result, specific heats could be measured at much lower temperatures, even as low as a few degrees above the absolute temperature minimum. In this way, it was discovered that the specific heat of solids decreases dramatically with decreasing temperature. It even appears to approach zero when the temperature approaches its absolute minimum.

The law of Dulong and Petit had been derived by utilizing classical physics, but it soon became clear that the laws of classical physics could not account for the behavior of specific heat at lower temperatures. It was Einstein who showed in 1907 that the application of the quantization concept explained the decrease in specific heat at lower temperatures. A subsequent more precise treatment by Debije produced a more accurate prediction of the temperature dependence of the specific heat in excellent agreement with experimental bindings.

Since the quantization concept led to a number of successful theoretical predictions, it became generally accepted. It played an important role in the next advance in the development of quantum mechanics, which was the result of problems related to the study of atomic structure.

## III. BOHR AND THE HYDROGEN ATOM

Atoms are too small to be studied directly, and until 1900 much of the knowledge of atomic structure had been obtained indirectly. Spectroscopic measurements made significant contributions in this respect.

An emission spectrum may be observed by sending an electric discharge through a gas in a glass container. This usually leads to dissociation of the gas molecules.

The atoms then emit the energy that they have acquired in the form of light of various frequencies. The emission spectrum corresponds to the frequency distribution of the emitted light.

It was discovered that most atomic emission spectra consist of a number of so-called spectral lines; that is, the emitted light contains a number of specific discrete frequencies. These frequencies could be measured with a high degree of accuracy.

The emission frequencies of the hydrogen atom were of particular interest. The four spectral lines in the visible part of the spectrum were measured in 1869 by the Swedish physicist *Anders Jöns Ångström* (1814–1874). It is interesting to note that the unit of length that is now commonly used for the wavelength of light is named after him. The Ångström unit (symbol Å) is defined as $10^{-8}$ cm. The wavelengths of the visible part of the spectrum range from 4000 to 8000 Å.

The publication of Ångström's highly precise measurements stimulated some interest in detecting a relationship between those numbers. In 1885 the Swiss physics teacher *Johann Jakob Balmer* (1825–1898) made the surprising discovery that the four wavelengths measured by Ångström could be represented exactly by the formular

$$\lambda = \frac{Am^2}{m^2 - 4} \qquad m = 3, 4, 5, 6 \tag{1-6}$$

A few years later, *Johannes Robert Rydberg* (1854–1919) proposed a more general formula

$$\nu = R\left(\frac{1}{n^2} - \frac{1}{m^2}\right) \quad n, m = 1, 2, 3 \quad (m > n) \tag{1-7}$$

which accurately represented all frequencies of the hydrogen emission spectrum, including those outside the visible part of the spectrum; $R$ became known as the Rydberg constant.

It was perceived first by Rydberg and later by *Walter Ritz* (1878–1909) that Eq. (1-7) is a special case of a more general formula that is applicable to the spectral frequencies of atoms in general. It is known as the combination principle, and it states that all the spectral frequencies of a given atom are differences of a much smaller set of quantities, defined as terms

$$\nu = \left| T_i - T_j \right| \tag{1-8}$$

We should understand that 10 terms determine 45 frequencies, 100 terms 4950 frequencies, and so on.

The above rules were, of course, quite interesting, and there was no doubt about their validity since they agreed with the experimental spectral frequencies to the many decimal points to which the latter could be measured. At the same time, there was not even the remotest possibility that they could be explained on the basis of the laws of classical physics and mechanics.

Meanwhile, a great deal of information about the structure of atoms had become available through other experiments. During a lecture on April 30, 1897 at the Royal Institution in Great Britain, *Joseph John Thomson* (1856–1940) first proposed the existence of subatomic particles having a negative electric charge and a mass considerably smaller than that of a typical atomic mass. The existence of these particles was confirmed by subsequent experiments, and they became known by the previously proposed name electrons.

Thomson's discovery of the electron was followed by a large number of experimental studies related to atomic structure. We will not describe these various discoveries in detail; suffice it to say that in May 1911 they helped *Ernest Rutherford* (1871–1937) propose a theoretical model for the structure of the atom that even today is generally accepted.

According to Rutherford, an atom consists of a nucleus with a radius of approximately $3 \times 10^{-12}$ cm, having a positive electric charge, surrounded by a number of electrons with negative electric charges at distances of the order of 1 Å ($10^{-8}$ cm) from the central nucleus. The simplest atom is hydrogen, where one single electron moves in an orbit around a much heavier nucleus.

Rutherford's atomic model has often been compared to our solar system. In a similar way, we may compare the motion of the electron around its nucleus in the hydrogen atom to the motion of the moon around the Earth. There are, however, important differences between the two systems. The moon is electrically neutral, and it is kept in orbit by the gravitational attraction of the Earth. It also has a constant energy since outside forces due to the other planets are negligible. The electron, on the other hand, has an electric charge, and it dissipates energy when it moves. According to the laws of classical physics, the energy of the electron should decrease as a function of time. In other words, the assumption of a stable electronic orbit with constant energy is inconsistent with the laws of classical physics. Since classical physics could not explain the nature of atomic spectra, the scientists were forced to realize that the laws of classical physics had lost their universal validity, and that they ought to be reconsidered and possibly revised.

The dilemma was solved by Niels Bohr, who joined Rutherford's research group in Manchester in 1912 after a short and unsatisfactory stay in Thomson's laboratory in Cambridge. Bohr set out to interpret the spectrum of the hydrogen atom, but in the process he made a number of bold assumptions that were developed into new fundamental laws of physics. His first postulate assumed the existence of a discrete set of stationary states with constant energy. A system in such a stationary state neither emits nor absorbs energy.

It may be interesting to quote Bohr's own words from a memoir he published in 1918:

> I. That an atomic system can, and can only, exist permanently in a certain series of states corresponding to a discontinuous series of values for its energy, and that consequently any change of the energy of the system, including emission and absorption of electromagnetic radiation, must take place by a complete transition between two such states. These states will be denoted as the "stationary states" of the system.

II. That the radiation absorbed or emitted during a transition between two stationary states is "unifrequentic" and possesses a frequency ν given by the relation

$$E' - E'' = h\nu$$

where $h$ is Planck's constant and where $E'$ and $E''$ are the values of the energy in the two states under consideration.

The second part of Bohr's statement refers to his second postulate, which states that a spectroscopic transition always involves two stationary states; it corresponds to a change from one stationary state to another. The frequency ν of the emitted or absorbed radiation is determined by Planck's relation $\Delta E = h\nu$. This second postulate seems quite obvious today, but it was considered revolutionary at the time.

Bohr successfully applied his theory to a calculation of the hydrogen atom spectrum. An important result was the evaluation of the Rydberg constant. The excellent agreement between Bohr's result and the experimental value confirmed the validity of both Bohr's theory and Rutherford's atomic model.

Bohr's hydrogen atom calculation utilized an additional quantum assumption, namely, the quantization of the angular momentum, which subsequently became an important feature of quantum mechanics. It should be noted here that Ehrenfest had in fact proposed this same correct quantization rule for the angular momentum a short time earlier in 1913. The rule was later generalized by Sommerfeld.

In the following years, Bohr introduced a third postulate that became known as the correspondence principle. In simplified form, this principle requires that the predictions of quantum mechanics for large quantum numbers approach those of classical mechanics.

Bohr returned to Copenhagen in 1916 to become a professor of theoretical physics. In that year Kramers volunteered to work with him, and Bohr was able to offer him a position as his assistant. Kramers worked with Bohr until 1926, when he was appointed to the chair of theoretical physics at the University of Utrecht in the Netherlands. Meanwhile, Bohr helped to raise funds for the establishment of an Institute for Theoretical Physics. He was always stimulated by discussions and personal interactions with other physicists, and he wanted to be able to accommodate visiting scientists and students. The Institute for Theoretical Physics was opened in 1921 with Bohr as its first director. During the first 10 years of its existence, it attracted over sixty visitors and became an international center for the study of quantum mechanics.

In spite of its early successes, the old quantum theory as it was practiced in Copenhagen between 1921 and 1925 left much to be desired. It gave an accurate description of the hydrogen atom spectrum, but attempts to extend the theory to larger atoms or molecules had little success. A much more serious shortcoming of the old quantum theory was its lack of a logical foundation. In its applications to atoms or molecules, random and often arbitrary quantization rules were introduced after the system was described by means of classical electromagnetic theory. Many physicists felt that there was no fundamental justification for these quantization rules other than the fact that they led to correct answers.

The situation improved significantly during 1925 and 1926 due to some dramatic advances in the theory that transformed quantum mechanics from a random set of rules into a logically consistent scientific discipline. It should be noted that most of the physicists listed in Table 1-1 contributed to these developments.

## IV. MATRIX MECHANICS

During 1925 and 1926 two different mathematical descriptions of quantum mechanics were proposed. The first model became known as matrix mechanics, and its initial discovery is attributed to Heisenberg. The second model is based on a differential equation proposed by Schrödinger that is known as the Schrödinger equation. It was subsequently shown that the two different mathematical models are equivalent because they may be transformed into one another. The discovery of matrix mechanics preceded that of the Schrödinger equation by about a year, and we discuss it first.

Matrix mechanics was first proposed in 1925 by Werner Heisenberg, who was a 23-year-old graduate student at the time. Heisenberg began to study theoretical physics with Sommerfield in Munich. He transferred to Göttingen to continue his physics study with Born when Sommerfeld temporarily left Munich to spend a sabbatical leave in the United States. After receiving his doctoral degree, Heisenberg joined Bohr and Kramers in Copenhagen. He became a professor of theoretical physics at Leipzig University, and he was the recipient of the 1932 Nobel Prize in physics at the age of 31.

Heisenberg felt that the quantum mechanical description of atomic systems should be based on physical observable quantities only. Consequently, the classical orbits and momenta of the electrons within the atom should not be used in a theoretical description because they cannot be observed. The theory should instead be based on experimental data that can be derived from atomic spectra. Each line in an atomic spectrum is determined by its frequency $\nu$ and by its intensity. The latter is related to another physical observable known as its transition moment. A typical spectral transition between two stationary states $n$ and $m$ is therefore determined by the frequency $\nu(n, m)$ and by the transition moment $x(n, m)$. Heisenberg now proposed a mathematical model in which physical quantities could be presented by sets that contained the transition moments $x(n, m)$ in addition to time-dependent frequency terms. When Heisenberg showed his work to his professor, Max Born, the latter soon recognized that Heisenberg's sets were actually matrices, hence the name matrix mechanics.

We present a brief outline of linear algebra, the theory of matrices and determinants in Chapter 2. Nowadays linear algebra is the subject of college mathematics courses taught at the freshman or sophomore level, but in 1925 it was an obscure branch of mathematics unknown to physicists. However, by a fortunate coincidence, linear algebra was the subject of the first chapter in the newly published book *Methods of Mathematical Physics* by Courant and Hilbert. *Ernst Pascual Jordan* (1902–1980) was Courant's assistant who helped write the chapter on

matrices, and he joined Born and Heisenberg in deriving the rigorous formulation of matrix mechanics. The results were published in a number of papers by Born, Jordan, and Heisenberg, and the discovery of matrix mechanics is credited to these three physicists.

We do not give a detailed description of matrix mechanics because it is rather cumbersome, but we attempt to outline some of its main features. In the classical description, the motion of a single particle of mass $m$ is determined by its position coordinates $(x, y, z)$ and by the components of its momentum $(p_x, p_y, p_z)$. The latter are defined as the products of the mass $m$ of the particle and its velocity components $(v_x, v_y, v_z)$:

$$p_x = mv_x, \text{ etc.} \tag{1-9}$$

Here $p_x$ is called conjugate to the coordinate $x$, $p_y$ to $y$, and $p_z$ to $z$. The above description may be generalized to a many-particle system by introducing a set of generalized coordinates $q_i$ and conjugate moments $p_i$. These generalized coordinates and momenta constitute the basis for the formulation of matrix mechanics.

In Chapter 2 we discuss the multiplication rules for matrices, and we will see that the product $\mathbf{A} \cdot \mathbf{B}$ of two matrices that we symbolically represent by the boldface symbols $\mathbf{A}$ and $\mathbf{B}$ is not necessarily equal to the product $\mathbf{B} \cdot \mathbf{A}$. In matrix mechanics the coordinates $q_i$ and moments $p_i$ are symbolically represented by matrices. For simplicity, we consider one-dimensional motion only. The quantization rule requires that the difference between the two matrix products $\mathbf{p} \cdot \mathbf{q}$ and $\mathbf{q} \cdot \mathbf{p}$ be equal to the identity matrix $\mathbf{I}$ multiplied by a factor $h/2\pi$. Since the latter combination occurred frequently, a new symbol $\hbar$ was introduced by defining

$$\hbar = h/2\pi \tag{1-10}$$

The quantization rule could therefore be written as

$$\mathbf{p} \cdot \mathbf{q} - \mathbf{q} \cdot \mathbf{p} = \hbar \cdot \mathbf{I} \tag{1-11}$$

In order to determine the stationary states of the system, it is first necessary to express the energy of the system as a function of the coordinate $q$ and the momentum $p$. This function is known as the Hamiltonian function $H$ of the system, and it is defined in Section 3.III. The matrix $\mathbf{H}$ representing the Hamiltonian is obtained by substituting the matrices $q$ and $p$ into the analytical expression for the Hamiltonian.

The stationary states of the system are now derived by identifying expressions for the matrix representations $\mathbf{q}$ and $\mathbf{p}$ that lead to a diagonal form for $\mathbf{H}$—in other words, to a matrix $\mathbf{H}$ where all nondiagonal elements are zero. The procedure is well defined, logical, and consistent, and it was successfully applied to derive the stationary states of the harmonic oscillator. However, the mathematics that is required for applications to other systems is extremely cumbersome, and the practical use of matrix mechanics was therefore quite limited.

There is an interesting and amusing anecdote related to the discovery of matrix mechanics. When Heisenberg first showed his work to Born, he did not know what matrices were and Born did not remember very much about them either, even though he had learned some linear algebra as a student. It was therefore only natural that they turned to Hilbert for help. During their meeting, Hilbert mentioned, among other things, that matrices played a role in deriving the solutions of differential equations with boundary conditions. It was this particular feature that was later used to prove the equivalence of matrix mechanics and Schrödinger's differential equation. Later on, Hilbert told some of his friends laughingly that Born and Heisenberg could have discovered Schrödinger's equation earlier if they had just paid more attention to what he was telling them. Whether this is true or not, it makes a good story. It is, of course, true that Schrödinger's equation is much easier to use than matrix mechanics.

## V.  THE UNCERTAINTY RELATIONS

Heisenberg's work on matrix mechanics was of a highly specialized nature, but his subsequent formulation of the uncertainty relations had a much wider appeal. They became known outside the scientific community because no scientific background is required to understand or appreciate them.

It is well known that any measurement is subject to a margin of error. Even though the accuracy of experimental techniques has been improved in the course of time and the possible errors of experimental results have become smaller, they are still of a finite nature. Classical physics is nevertheless designed for idealized situations based on the assumption that it is in principle possible to have exact knowledge of a system. It is then also possible to derive exact predictions about the future behavior of the system.

Heisenberg was the first to question this basic assumption of classical physics. He published a paper in 1927 where he presented a detailed new analysis of the nature of experimentation. The most important feature of his paper was the observation that it is not possible to obtain information about the nature of a system without causing a change in the system. In other words, it may be possible to obtain detailed information about a system through experimentation, but as a result of this experimentation, it is no longer the same system and our information does not apply to the original system. If, on the other hand, we want to leave the system unchanged, we should not disturb it by experimentation. Heisenberg's observation became popularly known as the uncertainty principle; it is also referred to as the indeterminacy principle.

Heisenberg summarized his observation at the conclusion of his paper as follows: ''In the classical law 'if we know the presence exactly we can predict the future exactly' it is the assumption and not the conclusion that is incorrect.''

A second feature of Heisenberg's paper dealt with the simultaneous measurement of the position or coordinate $q_i$ of a particle and of its conjugate momentum $p_i$. If, for example, we consider one-dimensional motion, it should be clear that we

must monitor the motion of a particle over a certain distance $\Delta q$ in order to deter-
mine its velocity $\upsilon$ and momentum $p$. It follows that the uncertainty $\Delta p$ in the result
of the momentum measurement is inversely related to the magnitude $\Delta q$; the larger
$\Delta q$ is the smaller $\Delta p$ is, and vice versa. Heisenberg now proposed that there should
be a lower limit for the product of $\Delta q$ and $\Delta p$ and that the magnitude of this lower
limit should be consistent with the quantization rule (1-11) of matrix mechanics.
The result is

$$\Delta q \cdot \Delta p > \hbar \qquad (1\text{-}12)$$

Heisenberg proposed a similar inequality for the uncertainty $\Delta E$ in measure-
ments of the energy of the system during a time interval $\Delta t$:

$$\Delta E \cdot \Delta t > \hbar \qquad (1\text{-}13)$$

It should again be obvious that the accuracy of energy measurements should
improve if more time is available for the experiment. The quantitative magnitude
of the lower limit of the product of $\Delta E$ and $\Delta t$ is consistent with the quantization
rules of matrix mechanics.

In Section 4.V, of Chapter 4, we describe a special situation that was created by
Heisenberg himself where the product of $\Delta q$ and $\Delta p$ is equal to $\hbar/2$, exactly half of
the value of the uncertainty relation (1-12). However, this is an idealized special
case, and it does not invalidate the principle of the uncertainty relations.

Heisenberg's work became of interest not only to physicists but also to philoso-
phers because it led to a reevaluation of the ideas concerning the process of mea-
surement and to the relations between theory and experiment. We will not pursue
these various ramifications.

## VI. WAVE MECHANICS

We have already mentioned that the formulation of wave mechanics was the next
important advance in the formulation of quantum mechanics. In this section we give
a brief description of the various events that led to its discovery, with particular
emphasis on the contributions of two scientists, Louis de Broglie and Erwin
Schrödinger.

Louis de Broglie was a member of an old and distinguished French noble family.
The family name is still pronounced as ''breuil'' since it originated in Piedmonte.
The family includes a number of prominent politicians and military heroes; two
of the latter were awarded the title ''Marshal of France'' in recognition of their
outstanding military leadership. One of the main squares in Strasbourg, the Place
de Broglie, and a street in Paris are named after family members.

Louis de Broglie was educated at the Sorbonne in Paris. Initially he was inter-
ested in literature and history, and at age 18 he graduated with an arts degree. How-
ever, he had developed an interest in mathematics and physics, and he decided to

pursue the study of theoretical physics. He was awarded a second degree in science in 1913, but his subsequent physics studies were then interrupted by the First World War. He was fortunate to be assigned to the army radiotelegraphy section at the Eiffel Tower for the duration of the war. Because of this assignment, he acquired a great deal of practical experience working with electromagnetic radio waves.

In 1920 Louis resumed his physics studies. He again lived in the family mansion in Paris, where his oldest brother, *Maurice, Duc de Broglie* (1875–1960), had established a private physics laboratory. Maurice was a prominent and highly regarded experimental physicist, and at the time he was interested in studying the properties of X rays. It is not surprising that the two brothers, Louis and Maurice, developed a common interest in the properties of X rays and had numerous discussions on the subject.

Radio waves, light waves, and X rays may all be regarded as electromagnetic waves. The various waves all have the same velocity of wave propagation $c$, which is considered a fundamental constant of nature and which is roughly equal to 300,000 km/sec. The differences between the types of electromagnetic waves are attributed to differences in wavelength. Visible light has a wavelength of about 5000 Å, whereas radio waves have much longer wavelengths of the order of 100 m and X rays have much shorter wavelengths of the order of 1 Å. The relation between velocity of propagation $c$, wavelength $\lambda$, and frequency $\nu$ is in all cases given by Eq. (1-2).

When Louis de Broglie resumed his physics studies in 1920, he became interested in the problems related to the nature of matter and radiation that arose as a result of Planck's introduction of the quantization concept. De Broglie felt that if light is emitted in quanta, it should have a corpuscular structure once it has been emitted. Nevertheless, most of the experimental information on the nature of light could be interpreted only on the basis of the wave theory of light that had been introduced by the Dutch scientist *Christiaan Huygens* (1629–1695) in his book *Traité de la Lumiere . . .* , published in 1690.

The situation changed in 1922, when experimental work by the American physicist *Arthur Holly Compton* (1892–1962) on X ray scattering produced convincing evidence for the corpuscular nature of radiation. Compton measured the scattering of so-called hard X rays (of very short wavelengths) by substances with low atomic numbers—for instance, graphite. Compton found that the scattered X rays have wavelengths larger than the wavelength of the incident radiation and that the increase in wavelength is dependent on the scattering angle.

Compton explained his experimental results by using classical mechanics and by describing the scattering as a collision between an incident X ray quantum, assumed to be a particle, and an electron. The energy $E$ and momentum $p$ of the incident X ray quantum are assumed to be given by

$$E = h\nu \qquad p = h\nu/c = h/\lambda \qquad (1\text{-}14)$$

The energy and momentum of the electron before the collision are much smaller than the corresponding energy $E$ and momentum $p$ of the X ray quantum, and

they are assumed to be negligible. Compton found that there was perfect agreement between his calculations and the experimental results. Maurice de Broglie quickly became aware of what is now popularly known as the Compton effect.

In a later memoir Louis remarked that in conversations with his brother, they concluded that X rays could be regarded both as particles and as waves. In his Nobel Prize lecture, Louis de Broglie explained that he felt that it was necessary to combine the corpuscular and wave models and to assume that the motion of an X ray quantum particle is associated with a wave. Since the corpuscular and wave motions cannot be independent, it should be possible to determine the relation between the two concepts.

Louis de Broglie's hypothesis assumed that the motion of an X ray was of a corpuscular nature and that the particle motion was accompanied by a wave. The relation between particle and wave motion was described by Eq. (1-14). De Broglie now proceeded to a revolutionary extension of this idea, namely, that the model was not confined to X rays and other forms of radiation but that it should be applicable to all other forms of motion, in particular the motion of electrons. Consequently, a beam of electrons moving with momentum $p$ should be associated with a wave with wavelength

$$\lambda = h/p \qquad (1\text{-}15)$$

De Broglie supported his proposal by a proof derived from relativity theory, but we will not present the details of this proof.

De Broglie described his theoretical ideas in his doctoral thesis with the title "Recherches sure la Théorie des Quanta," which he presented in November 1924 to the Faculty of Natural Science at the Sorbonne. The examination committee of the faculty had difficulty believing the validity of de Broglie's proposals, and one of its members asked how they could be verified experimentally. De Broglie answered that such verification might be obtained by measuring the pattern of diffraction of a beam of electrons by a single crystal. The committee was unaware of the fact that such experiments had already been performed. They nevertheless awarded the doctor's degree to Louis de Broglie because they were impressed by the originality of his ideas.

De Broglie was clearly not a member of the inner circle of prominent theoretical physicists centered at Munich, Göttingen, Berlin, and Copenhagen. However, Einstein was made aware of de Broglie's work. Upon his request, de Broglie sent Einstein a copy of his thesis, which the latter read in December 1924. Einstein brought the thesis to the attention of Max Born in Göttingen, who in turn described it to his colleague in experimental physics *James Franck* (1882–1964). Franck remembered that a few years earlier, two scientists at the AT&T Research Laboratories, *Clinton Joseph Davisson* (1881–1958) and *Charles Henry Kunsman* (1890–1970), had measured the scattering of a beam of electrons by a platinum plate. The experimental results exhibited some features that could be interpreted as a diffraction pattern. One of Born's graduate students, *Walter Maurice Elsasser* (1904–1991), calculated the diffraction pattern due to interference of de Broglie

waves associated with the electron beam and found that his theoretical result agreed exactly with the experiments. These results and subsequent diffraction measurements provided convincing experimental evidence for the validity of de Broglie's theories.

De Broglie received the 1929 Nobel Prize in physics, and we quote the words of the chairman of the Nobel Committee for Physics:

> When quite young you threw yourself into the controversy ranging round the most profound problem in physics. You had the boldness to assert, without the support of any known fact, that matter had not only a corpuscular nature, but also a wave nature. Experiment came later and established the correctness of your view. You have covered in fresh glory a name already crowned for centuries with honor.

De Broglie's theoretical model was primarily intended to describe the motion of free particles, but he also presented an application to the motion of an electron around a nucleus. In the latter case, it seems logical to assume that the circumference of the closed orbit should be equal to an integral number $n$ of de Broglie wavelength $h/p$. This requirement is identical to Sommerfeld's quantization rule mentioned in Section 1.III.

About a year after the publication of de Broglie's thesis, Erwin Schrödinger formulated the definitive mathematical foundation of quantum mechanics in a series of six papers that he wrote in less than a year during 1926. The key feature of this model, the Schrödinger equation, has formed the basis for all atomic and molecular structure calculations ever since it was first proposed, and it is without doubt the best-known equation in physics.

There are actually two Schrödinger equations, the time-independent equation

$$-\frac{\hbar^2}{2m}\Delta\psi + V\psi = E\psi \tag{1-16a}$$

and the time-dependent one

$$-\frac{\hbar^2}{2m}\Delta\psi + V\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t} \tag{1-16b}$$

The two equations are closely related.

The symbol $\Delta$ denotes the Laplace operator:

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial x^2} \tag{1-17}$$

and the symbol $V$ represents the potential energy. The above are one-particle Schrödinger equations, but their generalization to larger systems containing more particles is quite straightforward.

We shall see that for positive values of energy $E$, the Schrödinger equation describes the motion of a free or quasi-free particle. In the case of bound particles

whose motion is confined to closed orbits of finite magnitude, additional restraints must be imposed on the solutions of the equations. Mathematicians classify the Schrödinger equation as a partial differential equation with boundary conditions that is similar in nature to the problem of a vibrating string. Schrödinger had received an excellent education in mathematics, and he was familiar with this particular topic.

Erwin Schrödinger was the most interesting of the physicists listed in Table 1-1, since he had both a fascinating personality and an interesting life. He was born in 1887 into a comfortable upper-middle-class family in Vienna, where his father owned a profitable business. He had a happy childhood. He was the top student at the most prestigious type of high school, the gymnasium, that he attended. He also took full advantage of the lively cultural atmosphere in Vienna at the time; he particularly liked the theatre. At school he was interested in literature and philosophy, but he decided to study theoretical physics and enrolled at the University of Vienna in 1906.

Erwin's academic studies in physics proceeded smoothly. He received an excellent education in mathematical physics and was awarded a doctor's degree in 1910. In order to satisfy his military obligations, he volunteered for officer's training and served for 1 year (1910–1911), after which he joined the army reserve. He returned to the university in 1911, and in 1914 he was admitted to the faculty of the University of Vienna as a *Privatdozent*. This meant that he was allowed to conduct research and give lectures at the university, but he did not necessarily receive any salary in return.

Schrödinger's academic career, like that of Louis de Broglie, was rudely interrupted by the outbreak of the First World War in 1914. Schrödinger was recalled to military duty and served as an artillery officer at the southern front until 1917. At that time he was reassigned as a meteorology officer in the vicinity of Vienna since he had taken a course in meteorology as a student. This transfer may very well have saved his life.

After the war Schrödinger returned home to Vienna, where he found that living conditions were quite bleak. This should not have come as a surprise; after all, Austria had lost the war. His father's business had failed as a result of the war and his savings had been eroded due to inflation, so the financial conditions of the family were far from favorable. His health also deteriorated, and he died towards the end of 1919.

During that time Erwin received a small stipend from the university, and even though this was inadequate to meet his living expenses, he worked very hard at research. His main interest was the theory of color, a subject that straddled physics, physiology, and psychology. He wrote a number of research papers on the subject followed by a highly regarded review.

Schrödinger's academic career took a turn for the better in 1920, when he was offered a low-level faculty position at the University of Jena. He did not stay there very long because, like most other professors, he was interested in finding a better job at a more prestigious university. In the next few years he moved first to Stuttgart, then to Breslau, and finally, in 1921, to Zürich, where he was appointed

a full professor of theoretical physics at a generous annual salary of 14,000 SFr. He had found an excellent academic position away from the political and economic turmoil of Germany and Austria.

At the time of his appointment, Schrödinger could be considered a typical average physics professor. He was highly knowledgeable and he had published a number of competent research papers, but his name was not associated with any major discovery. He was probably best known for his work on the theory of color.

In addition to the University of Zürich, there is also a technical university in the city, the Eidgenössische Technische Hochschule (E.T.H.), which was regarded as the more prestigious of the two. The physics professor at the E.T.H. was the Dutchman Pieter Debije, who was better known and more highly regarded than Schrödinger at the time. The two physics professors met frequently at their joint physics seminar.

It was Debije who first became aware of de Broglie's work and who brought it to Schrödinger's attention. De Broglie's thesis had been published in a French physics journal, and Debije suggested that Schrödinger give a seminar in order to explain it to the Zürich physicsts. After the seminar Schrödinger realized that in classical physics waves were usually interpreted as solutions of a partial differential equation, the so-called wave equation. It occurred to him that it might be possible to formulate a similar wave equation for the description of de Broglie waves, and he set out to try to derive such a wave equation.

At first Schrödinger tried to derive a wave equation by using relativity theory. Even though he was successful, the results of this equation did not agree with the experimental information on the hydrogen atom's spectrum. This lack of agreement could probably be attributed to effects of the electron spin, which had not yet been discovered. Schrödinger nevertheless changed his approach, and he derived a wave equation based on classical nonrelativistic mechanics.

During the next 6 months, the first half of the year 1926, Schrödinger wrote six research papers in which he presented the complete mathematical foundation of nonrelativistic quantum mechanics. In fact, the contents of this book are based almost entirely on the six Schrödinger papers.

Schrödinger's wave equation bears some resemblance to the equation describing the motion of a vibrating string. The mathematicians classify it as a partial differential equation with boundary conditions. The solutions of the differential equation are required to assume specific values at various points. This condition is satisfied only for a discrete set of values of a parameter in the equation. The German word for these values is *Eigenwerte*, which has been translated in English as eigenvalues rather than the more suitable term specific values. This particular problem is also known among mathematicians as the Sturm-Liouville problem.

In the Schrödinger equation, the adjustable parameter is the energy and its eigenvalues correspond to the quantized stationary states for the system. In addition to proposing the equation, Schrödinger derived its solution for a variety of systems, including the hydrogen atom. He accomplished this during a 6-month period of intense concentration, a truly spectacular effort.

Schrödinger remained in Zürich until 1927, when he received an offer to become Planck's successor at the University of Berlin. The offer was hard to resist because the position was not only very lucrative but also extremely prestigious; the second chair of theoretical physics at the university was held by Einstein. Also, Berlin was a vibrant and attractive city at the time. Schrödinger had won what was probably the best academic job in Europe just before his fortieth birthday. All went well until 1933, when the Nazis under the leadership of Adolf Hitler came to power and introduced a succession of anti-Jewish laws. Einstein happened to be in the United States at the beginning of 1933, and he decided not to return to Germany. Schrödinger had never been particularly interested in politics, but in this instance he decided that he no longer wanted to stay in Germany. He moved to Oxford, where he became a Fellow of Magdalen College. He did not formally resign his professorship, but he requested a leave of absence and sent a postcard to the physics department to inform the students that his lectures for the fall semesters would be canceled. He did not make a dramatic exit; he just left.

During the next few years, Schrödinger traveled widely. He received the 1933 Nobel Prize in physics, and he was in great demand as a guest lecturer. He also had to find a permanent academic position since his appointment in Oxford was temporary. He had the choice of a number of academic positions, but he made an almost fatal error in accepting a professorship at the University of Graz in his native Austria. When the Austrian Nazis managed to arrange a merger with Germany, the so-called *Annschluss*, Schrödinger found himself suddenly in a very precarious position since his departure from Germany had deeply offended the Nazis. He was fortunate to be able to leave the country without being arrested, but he had to leave all his possessions, including his money and valuables, behind.

The president of Ireland invited Schrödinger to become the director of a newly established institute for theoretical physics in Dublin, where he spent the next 18 years. In 1956, when Schrödinger's health was already beginning to fail, he moved back to his native Vienna as a professor of physics. He died there in 1961.

## VII. THE FINAL TOUCHES OF QUANTUM MECHANICS

In Schrödinger's work the emphasis was on the energy eigenvalues, the discrete values of the energy parameter that correspond to acceptable solutions of the differential equation. It was shown that these eigenvalues coincide with the energies of Bohr's stationary states. Much less attention was paid to the physical interpretation of solutions of the equation corresponding to each eigenvalue; these latter functions became known as eigenfunctions.

It was Born who proposed in the same year, 1926, that the product of an eigenfunction $\psi$ and its complex conjugate $\psi^*$ represents the probability density of the particle. In other words, the probability of finding the particle in a small-volume element surrounding a given point is given by the product of the volume element and the value of the probability density $\psi \cdot \psi^*$ at that point.

Born's interpretation is easily extended to situations where a one-particle system is described by a wave function $\psi(x, y, z, t)$ that may or may not be an eigenfunction corresponding to a stationary state. Here the product $\psi \cdot \psi^*$ is again a representation of the probability density of the particle. Even though quantum mechanics does not offer an exact prediction of the position of the particle, it offers an exact prediction of the statistical probability distribution of locating the particle.

Born first proposed the probabilistic interpretation of the wave function in relation to a theory of electron scattering, in particular the scattering of a high-energy electron by an atom. He later extended the idea to all other aspects of quantum mechanics, and it became universally accepted. Born's statistical interpretation of the wave function is probably the most important of his many contributions to the development of quantum mechanics. The award of the 1954 Nobel Prize in physics to Max Born at age 72 was motivated primarily by this contribution.

The formal description of quantum mechanics as we know it today was completed in just a few years. We briefly describe the various developments. The motion of an electron around a nucleus in an atom has often been compared to the motion of the planets around the sun. We know that the Earth not only describes an annual orbit around the sun but also performs a diurnal rotation around its axis. The idea occurred to two graduate students at Leiden University, *George Uhlenbeck* and *Samuel Goudsmit*, that by analogy, the electron might also be capable of rotational motion around its axis. At the time, there were certain features in atomic spectra (referred to as the anomalous Zeeman effect) that defied all logical explanation. Goudsmit and Uhlenbeck proposed in 1925 that the assumption of rotational motion within the electron and subsequent quantization of this motion offered the possibility of explaining the anomalous Zeeman effect. The rotational motion of the electron became known as the electron spin. Goudsmit and Uhlenbeck's theory led to perfect agreement with the experimental atomic spectral features.

Initially Goudsmit and Uhlenbeck's ideas were severely criticized because they appeared to be inconsistent with classical electromagnetic theory. However, early in 1926, *Lewellyn Hilleth Thomas* (1903–1992) showed that Goudsmit and Uhlenbeck's assumptions were entirely correct if the relativistic effect was taken into account.

The theoretical description of the spinning electron became a fundamental aspect of quantum mechanics when Paul Dirae generalized the Schrödinger equation to make it consistent with relativity theory. The existence of the electron spin was an essential feature of the Dirae equation. We should add that relativistic quantum mechanics is not included in this book since we believe it to be too sophisticated for our level of presentation.

The Schrödinger equation is easily extended to many-electron systems, but in that case the wave function is subject to an additional restraint due to the Pauli exclusion principle. In interpreting the electronic structure of an atom, it had been customary to assign each electron for identification purposes to a stationary state determined by a set of quantum numbers. In order to be consistent with the experimental information on atomic structure, Wolfgang Pauli imposed in 1925 the condition that no more than two electrons could be assigned to the same stationary

state. When the spin is included in the definition of the stationary state, no more than one electron can be assigned to each state. This condition became known as the Pauli exclusion principle. We will present a more general and more exact formulation of the exclusion principle when we discuss the helium atom in Chapter 10.

The mathematical formalism of quantum mechanics was completed in 1927, and all that remained was to find solutions to the Schrödinger equation for atomic and molecular systems. This required the introduction of approximate techniques since exact analytical solutions could be derived only for a limited number of one-particle systems. Today, highly accurate solutions of the Schrödinger equation for relatively large molecules can be obtained. This is due to the concerted effort of many scientists and also to the introduction of high-speed computers. We may conclude that the majority of the problems involving the application of quantum mechanics to atomic and molecular structure calculations have been solved.

## VIII. CONCLUDING REMARKS

Quantum mechanics is basically a conglomerate of revolutionary new ideas and concepts. The most important of these are Planck's quantization, Bohr's introduction of stationary states, Heisenberg's uncertainty relations, de Broglie's wave-particle duality, Schrödinger's equation, and Born's statistical interpretation of the wave function. Dirac remarked in his textbook that these new theoretical ideas are built up from physical concepts that cannot be explained in terms of things previously known to the student and that cannot be explained adequately in words at all. They definitely cannot be proved.

It is best to look upon them as new fundamental laws of physics that form a logically consistent structure and that are necessary to interpret all known experimental facts.

We have made a deliberate attempt to present these novel ideas from a non-mathematical perspective. Unfortunately, it is not possible to apply the ideas without making use of mathematical techniques. We present the necessary background material in the following two chapters.