Wave Properties of Matter

I thus arrived at the following overall concept which guided my studies: for both matter and radiations, light in particular, it is necessary to introduce the corpuscle concept and the wave concept at the same time.

Louis de Broglie, 1929

C hapter 3 presented compelling evidence that light (electromagnetic radiation) must be particlelike in order to explain phenomena such as the photoelectric effect and Compton scattering. The emission and absorption of photons in atoms allow us to understand the optical spectra of hydrogen atoms.

In this chapter we will learn another surprising result: wavelike properties are also exhibited by "particles" of matter. This is the only way we can interpret certain experimental observations. We begin the chapter by discussing experiments that prove that photons, in the form of x rays, behave as waves when passing through crystals. De Broglie's suggestion that particles may also behave as waves was verified by the electron-scattering experiments of Davisson and Germer.

We then present a short review of wave phenomena, including a description of the localization of a particle in terms of a collection of waves. A major hurdle is to understand how wavelike and particlelike properties can occur in nature in the same entity. Niels Bohr's principle of complementarity convinces us that *both* wavelike and particlelike properties are needed to give a complete description of matter (electrons, protons, etc.) and radiation (photons). We shall see that certain physical observables can only be determined from probabilities by using wave functions $\Psi(x, t)$. Heisenberg's uncertainty principle plays a major role in our understanding of particlelike and wavelike behavior. This principle prohibits the precise, simultaneous knowledge of both momentum and position or of both energy and time. We will see that no experiment exhibits both wave and particle properties *simultaneously*. Although modern quantum theory is applicable primarily at the atomic level, there are many macroscopic observations of its effects.

5.1   X-Ray Scattering

Following Roentgen's discovery of x rays in 1895, intense efforts were made to determine the nature and origin of the new penetrating radiation. Charles Barkla (Nobel Prize, 1917) made many x-ray measurements at Liverpool University during the early 1900s and is given credit for discovering that each element emits x rays of characteristic wavelengths and that x rays exhibit properties of polarization.

By 1912 it became clear that x rays were a form of electromagnetic radiation and must therefore have wave properties. However, because it had proved difficult to refract or diffract x rays as easily as visible light, it was suggested that their wavelengths must be much shorter than those of visible light. Max von Laue (1879–1960), a young theoretical physicist at the University of Munich, became interested in the nature of x rays primarily because of the presence at Munich of Roentgen and the theorist Arnold Sommerfeld (1868–1951), who would later play an important role in understanding atomic structure. Wilhelm Wien (1864–1928) and Sommerfeld, among others, estimated the wavelength of an x ray to be between 10^{-10} and 10^{-11} m. Knowing the distance between atoms in a crystal to be about 10^{-10} m, von Laue made the brilliant suggestion that x rays should scatter from the atoms of crystals and, if x rays were a form of electromagnetic radiation, interference effects should be observed. From the study of optics, we know that wave properties are most easily demonstrated when the sizes of apertures or obstructions are about equal to or smaller than the wavelength of the light. Von Laue suggested that crystals may act as three-dimensional gratings, scattering the waves and producing observable interference effects.

Max von Laue (Nobel Prize, 1914) designed the experiment and convinced two experimental physicists at Munich, Walter Friedrich and Paul Knipping, to perform the measurement. A schematic diagram of the transmission Laue process is shown in Figure 5.1, along with one of Friedrich and Knipping's earliest experimental results. By rotating the crystals, the positions and intensities of
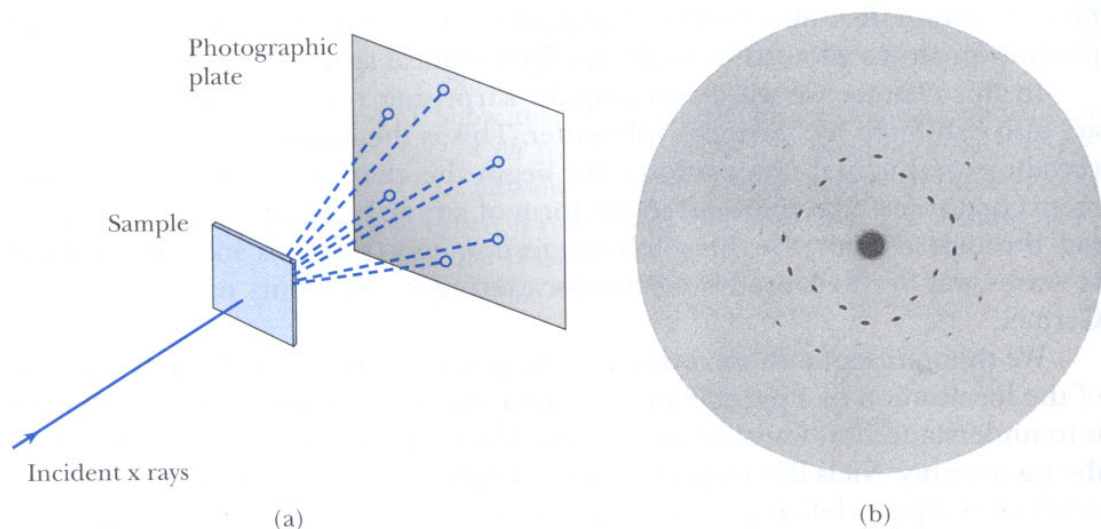

Photographic plate

Sample

Incident x rays

(a)   (b)

FIGURE 5.1   (a) Schematic diagram of Laue diffraction transmission method. A wide range of x-ray wavelengths scatter from a crystal sample. The x rays constructively interfere from certain planes producing dots. (b) One of the first results of Friedrich and Knipping in 1912 showing the symmetric placement of *Laue dots* of x-ray scattering from ZnS. The analysis of these results by von Laue, although complex, convincingly proved that x rays are waves. *Photo from W. Friedrich, P. Knipping, and M. Laue, Sitzungsberichte der Bayerischen Akademie der Wissenschaften (1912), 303–322 und 5 Tafeln, reprinted in Max von Laue, Gesammelte Schriften und Vorträge, Band 1, Vieweg & Sohn, Braunschweig, 1961.*
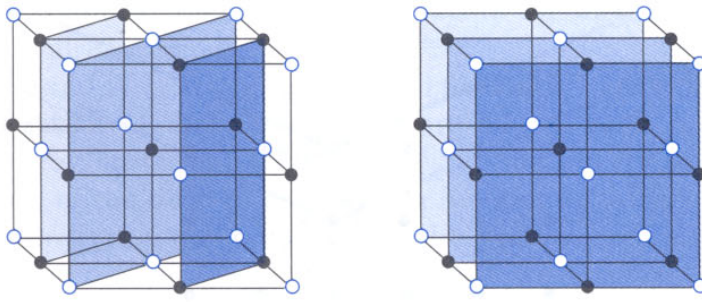
FIGURE 5.2 The crystal structure of NaCl (rock salt) showing two of the possible sets of lattice planes (Bragg planes).

the diffraction maxima were shown to change. Von Laue was able to perform the complicated analysis necessary to prove that x rays were scattered as waves from a three-dimensional crystal grating. We emphasize that von Laue was able to prove convincingly not only the wave nature of x rays but also the lattice structure of crystals.

Proof of wave nature of x rays and lattice theory of crystals

Two English physicists, William Henry Bragg and his son, William Lawrence Bragg, fully exploited the wave nature of x rays and simplified von Laue's analysis. W. L. Bragg pointed out in 1912 that each of the images surrounding the bright central spot of the Laue photographs could be interpreted as the reflection of the incident x-ray beam from a unique set of planes of atoms within the crystal. Each dot in the pattern corresponds to a different set of planes in the crystal (see Figure 5.1b).

Is x-ray scattering from atoms within crystals consistent with what we know from classical physics? From classical electromagnetic theory we know that the oscillating electric field of electromagnetic radiation polarizes an atom, causing the positively charged nucleus and negatively charged electrons to move in opposite directions. The result is an asymmetric charge distribution, or electric dipole. The electric dipole oscillates at the same frequency as the incident wave and in turn reradiates electromagnetic radiation at the same frequency, but in the form of spherical waves. These spherical waves travel throughout the matter and, in the case of crystals, may constructively or destructively interfere as the waves pass through different directions in the crystal.

If we consider x rays scattered from a simple rock salt crystal (NaCl, shown in Figure 5.2), we can, by following the Bragg simplification, determine conditions necessary for constructive interference. We will study solids in Chapter 10, but for now, note that the atoms of crystals, like NaCl, form lattice planes, called **Bragg planes.** We can see from Figure 5.3 that it is possible to have many Bragg
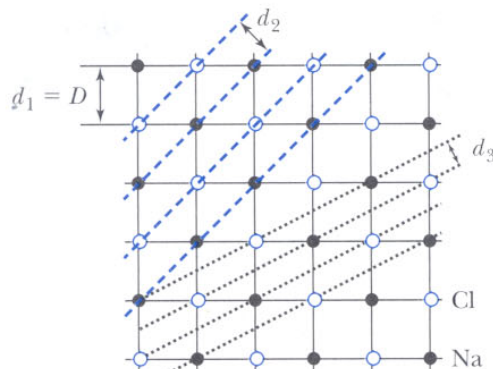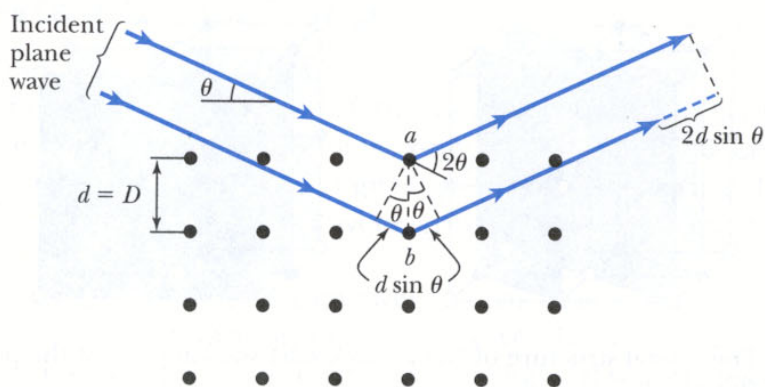

FIGURE 5.3 Top view of NaCl (cubic crystal), indicating possible lattice planes.

FIGURE 5.4 Schematic diagram illustrating x-ray scattering from Bragg lattice planes. The path difference of the two waves illustrated is $2d \sin \theta$. Notice that the actual scattering angle from the incident wave is 2θ.

planes in a crystal, each with different densities of atoms. Figure 5.4 shows an incident plane wave of monochromatic x rays of wavelength λ scattering from two adjacent planes. There are two conditions for constructive interference of the scattered x rays:

Conditions for constructive interference

1. The angle of incidence must equal the angle of reflection of the outgoing wave.
2. The difference in path lengths shown in Figure 5.4 ($2d \sin \theta$) must be an integral number of wavelengths.

We will not prove condition 1 but will assume it.* It is referred to as the *law of reflection* ($\theta_{incidence} = \theta_{reflection}$), although the effect is actually due to diffraction and interference. Condition 2 will be met if

Bragg's law

$$n\lambda = 2d \sin \theta \qquad n = \text{integer} \tag{5.1}$$

as can be seen from Figure 5.4, where D is the interatomic spacing (distance between atoms) and d is the distance between lattice planes. Equation (5.1) was first presented by W. L. Bragg in 1912 after he learned of von Laue's results. The integer n is called the *order of reflection*, following the terminology of ruled diffraction gratings in optics. Equation (5.1) is known as **Bragg's law** and is useful

*See L. R. B. Elton and D. F. Jackson, *Am. J. Phys.* **34,** 1036 (1966), for a correct proof.
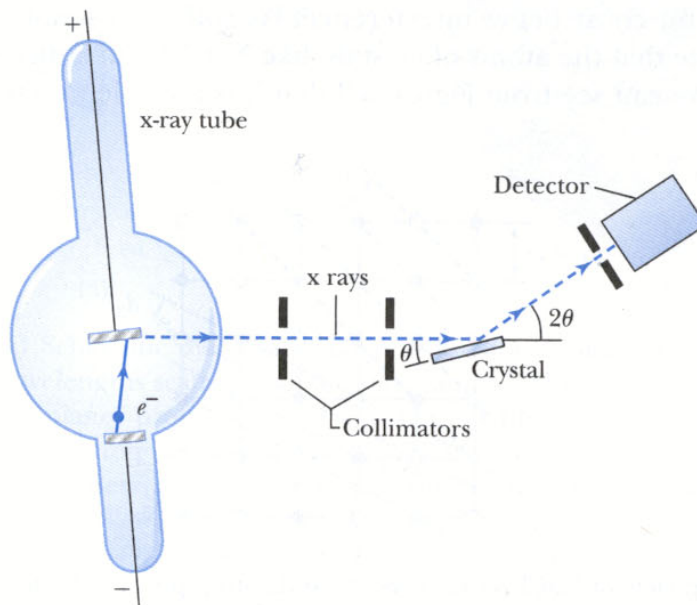

FIGURE 5.5 Schematic diagram of Bragg spectrometer. X rays are produced by electron bombardment of metal target. The x rays are collimated by lead and scatter from a crystal and are detected as a function of the angle 2θ.

for determining either the wavelength of x rays or the interplanar spacing d of the crystal if λ is already known.

W. H. Bragg and W. L. Bragg (who shared the 1915 Nobel Prize) constructed an apparatus similar to that shown in Figure 5.5, called a *Bragg spectrometer,* and scattered x rays from several crystals. By rotating the crystal and the detector, the intensity of the diffracted beam as a function of scattering angle is determined. The Braggs' studies opened up a whole new area of research that continues today.

The Bragg and Laue methods are complementary. In the Bragg method, the crystal is normally placed so that a certain set of planes produces constructive interference. The Bragg method is best for measuring x-ray wavelengths, and monochromatic x rays usually are used. The Laue method emphasizes x-ray transmission and is best for actually studying the crystal structure. Each of the symmetric Laue dots represents planes for which the two Bragg conditions are fulfilled. This technique of studying crystals is widespread, and many incident wavelengths normally are used simultaneously in order to obtain many dots. These techniques tell us almost everything we know about the structures of solids, liquids, and even complex molecules such as DNA.

There is still another possibility for study, although more than just a brief mention of the process is beyond the level of this text. If a single large crystal is not available, then many small crystals may be used. If these crystals are ground into a powdered form, the small crystals will then each have random orientations. Because of random orientations, when a beam of x rays passes through the powdered crystal, the dots become a series of rings. A schematic diagram of the *powder technique* is shown in Figure 5.6a along with the film arrangement to record powder photographs in Figure 5.6b. The lines indicated in part (b) are sections of rings called the *Debye-Scherrer pattern,* named after the discoverers. Figure 5.6c is a sequence of four photographs, each with an increasingly larger number of crystals, which indicates the progression from the Laue dots to the rings characteristic of the powder photographs.
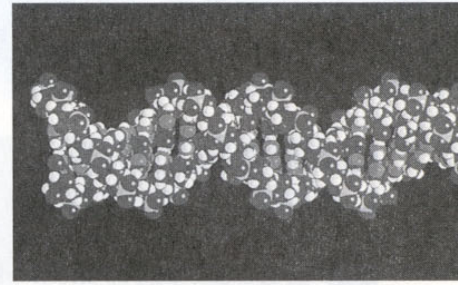
A computer graphic of the DNA double helix is shown. This complex structure was understood only after hundreds of x-ray diffraction photos were carefully studied. *Copyright Nelson Max/LLNL, Peter Arnold, Inc.*
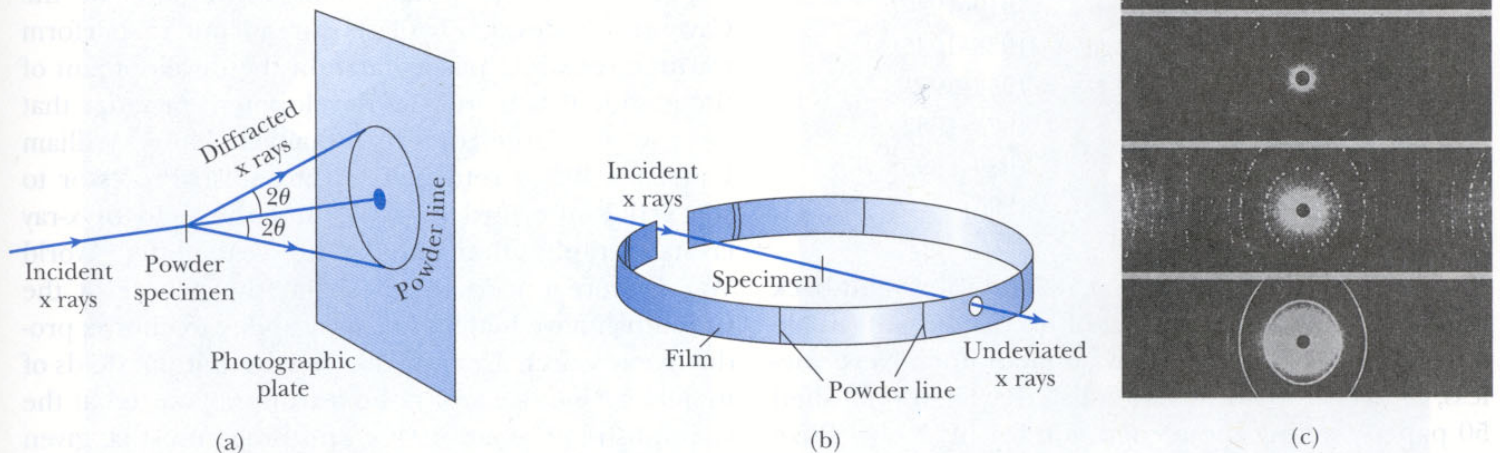
FIGURE 5.6 (a) Diagram showing the experimental arrangement of producing powder photographs from random-oriented crystals. (b) Film arrangement to record powder photographs. (c) The four photos show a progression of x-ray photographs for fluorite from a single crystal (clearly showing dots), through a few crystals, to a large number of crystals, which gives the rings the characteristic of an ideal powder photograph. *(a) and (b) are taken from N. F. M. Henry, H. Lipson, and W. A. Wooster, The Interpretation of X-ray Diffraction Photographs. London: MacMillan, 1960. (c) is from H. S. Lipson, Crystals and X-Rays. London: Wykeham Publications, 1970.*

CAVENDISH LABORATORY

Before the 1870s most of our scientific knowledge resulted from the research of persons working in their own private laboratories or in a private college room. Lord Kelvin established a laboratory at Glasgow in the 1840s, and in the 1860s efforts began at both Oxford and Cambridge to build physical laboratories. In 1871 James Clerk Maxwell was called from his Scottish home to become the first Cavendish Professor. Maxwell began planning and supervising the construction of the laboratory on Free School Lane in central Cambridge with an unexpected fervor while he gave regular lectures to students. The publication of Maxwell's treatise on electricity and magnetism in 1873 made him famous. The most important work of the day was to demonstrate the existence of Maxwell's electromagnetic waves, but they were "scooped" by Heinrich Hertz in Germany. However, the Cavendish research on waves was extensive and productive. Maxwell died in 1879, and his successor was Lord Rayleigh, a famous physicist who had not yet done his most important work. The line of Cavendish professors is impressive:

James Clerk Maxwell	1871–1879
Lord Rayleigh	1879–1884
Sir J. J. Thompson	1884–1919
Lord Rutherford	1919–1937
Sir W. Lawrence Bragg	1938–1953
Sir Nevill Mott	1954–1971
Sir Brian Pippard	1971–1982
Sir Sam Edwards	1984–1995
Richard H. Friend	1995–

Rayleigh remained only five years and then went back to his estate farm where most of his discoveries (noble gases) were made at his private laboratory. Nevertheless, in his five years at Cavendish, Rayleigh published 50 papers, setting the recognition for his Nobel Prize of 1904.

The appointment of the young J. J. Thomson at age 28 as Cavendish Professor in 1884 was the beginning of a long and fruitful era in atomic physics. The discovery of the electron in 1897, the arrival of the young Ernest Rutherford from New Zealand as a student, and the early work of C. T. R. Wilson that led to the development of the cloud chamber all helped the Cavendish Laboratory expand, prosper, and grow in stature under Thomson's leadership. Young William Lawrence Bragg started his Nobel Prize–winning research as a Cavendish student in 1912 with his father who was then a Professor of Physics at Leeds. Thomson's 35-year leadership was remarkable in many ways, particularly in the manner he stepped down in 1919 upon the opportunity of attracting Rutherford back to Cavendish to be the next Professor.

During Rutherford's 19-year reign, the Cavendish became the most renowned center of science in the world. It attracted the best students and researchers and received visitors from all over the world. Rutherford was a team leader, and he surrounded himself with a collection of young physicists whom he called "his boys." Lectures by Thomson on "Conduction of Electricity in Gases," by F. W. Aston on isotopes, by Chadwick on the discovery of the neutron, by P. M. S. Blackett on nuclear disintegration, and reports on the research of Cockcroft and Walton were on the forefront of physics. By the end of the Rutherford era in 1937, the laboratory was moving into new directions with particle accelerators and cryogenic labs. In one year, 1927–1928, the Cavendish published 53 papers.

World War II would change the face of the Cavendish forever. Physicists spread out to perform wartime research, particularly on the development of the atomic bomb and the development of radar that were to play large roles in the allied victory. William Lawrence Bragg returned as Cavendish Professor to succeed Rutherford in 1937, and the field of x-ray crystallography flourished. The years after World War II were uncertain ones, but the people at the Cavendish have had an uncanny ability to choose productive research areas. It can be said that the fields of molecular biology and radio astronomy started at the Cavendish in the late 1940s, and Bragg must be given credit for the foresight in supporting these fledgling subjects in the face of "Big Science" in the United States. Bragg's tenure as Cavendish Professor ended in 1953 just when Watson and Crick succeeded in dis-
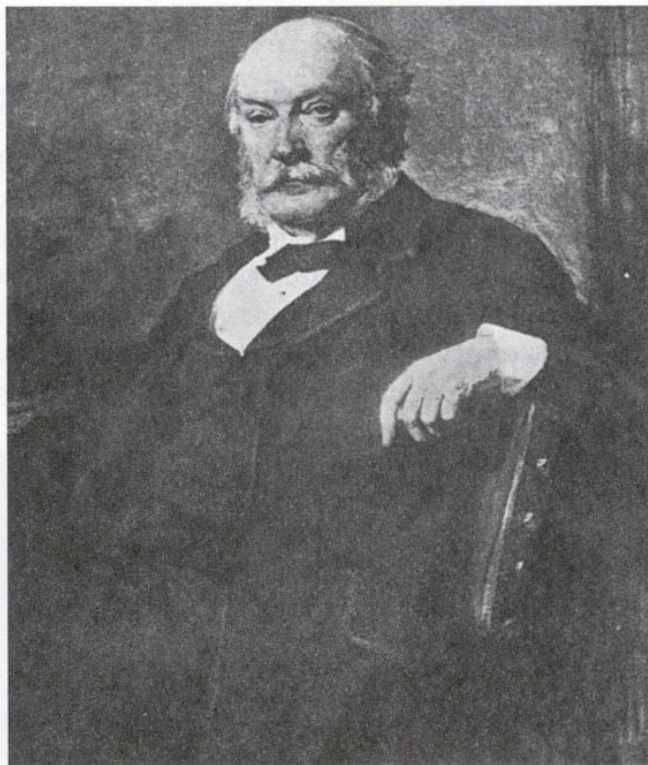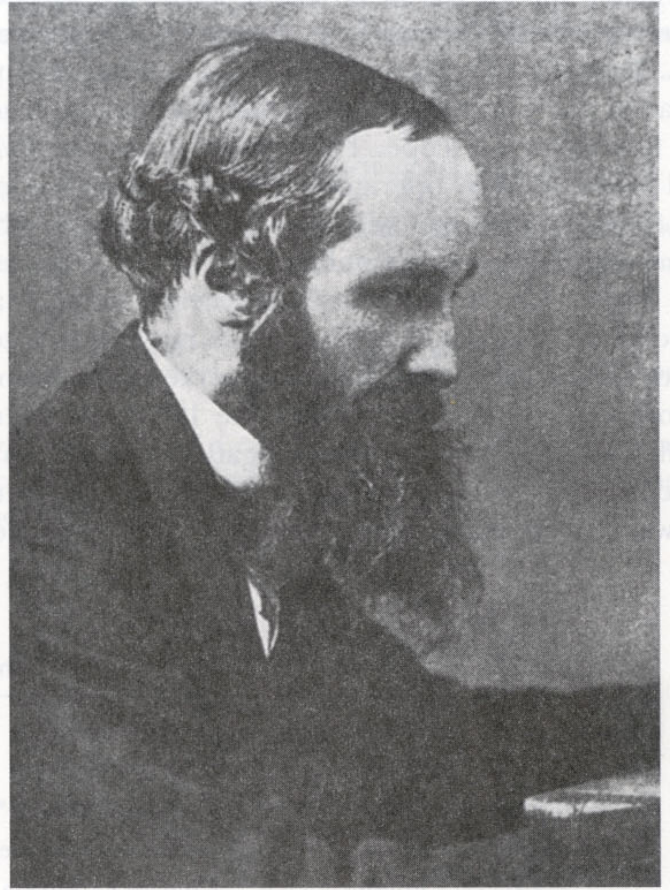
In the upper left photo is shown the old Cavendish Laboratory on Free School Lane in Cambridge. The original building is to the left of the gate. Pictured are also the first four Cavendish Professors, James Clerk Maxwell in the upper right, Lord Rayleigh in the bottom left, and Sir J. J. Thomson (left) and Lord Rutherford in the bottom right.

covering the DNA structure. Bragg also supported J. A. Ratcliffe and Martin Ryle, who had worked on radar at the Cavendish during the war, to construct the first radio telescope. This occurred because Ryle had heard of radar operators' reports of signals coming from the stars and galaxies. This effort led to the discovery of quasars and pulsars.

When Sir Neville Mott succeeded Bragg as Cavendish Professor in 1954, the lab made a turn towards solid state physics. Mott had worked on collision theory and nuclear problems in the 1930s, but eventually turned to theoretical investigations of electronic systems. Brian Josephson did his pioneering theoretical work on the supercurrent through a tunnel barrier while a student, graduating in 1964 with his Ph.D. In 1974 the Cavendish moved to a new site in West Cambridge. Condensed matter physics now accounts for the greater part of research at the Cavendish, but the groups in radio astronomy and high energy physics are still important.

We end with a list of Nobel Prizes awarded to those who did their most important work at the Cavendish Laboratory. The asterisks (for example, Rutherford and Rayleigh) indicate examples where the Nobel Prizes were awarded primarily for work done elsewhere, but those persons are still widely associated with the Cavendish Laboratory.

Cavendish Laboratory Nobel Prizes

Year	Field	Laureate	Work
1904	Physics	Lord Rayleigh*	Density of gases, discovery of argon
1906	Physics	Sir J. J. Thomson	Investigations of electricity in gases
1908	Chemistry	Lord Rutherford*	Element disintegration
1915	Physics	Sir William Lawrence Bragg	X-ray analysis of crystals
1917	Physics	Charles G. Barkla	Secondary x rays
1922	Chemistry	Francis W. Aston	Isotopes discovery
1927	Physics	Charles T. R. Wilson	Cloud chamber
1928	Physics	Sir Owen W. Richardson	Thermionic emission
1935	Physics	Sir James Chadwick	Neutron discovery
1937	Physics	Sir George P. Thomson	Electron diffraction
1947	Physics	Sir Edward V. Appleton*	Upper atmosphere investigations
1948	Physics	Lord Patrick M. S. Blackett	Discoveries in nuclear physics
1951	Physics	Sir John D. Cockcroft and Ernest T. S. Walton	Nuclear transmutation
1962	Physiology or Medicine	Francis H. C. Crick and James D. Watson	DNA discoveries
1973	Physics	Brian D. Josephon	Supercurrent in tunnel barriers
1974	Physics	Sir Martin Ryle and Anthony Hewish	Radio astrophysics, pulsars
1977	Physics	Sir Nevill F. Mott	Magnetic and disordered systems
1978	Physics	P. L. Kapitsa*	Low temperature physics
1982	Chemistry	Sir Aaron Klug	Nuclei acid protein complexes

Example 5.1

X rays scattered from rock salt (NaCl) are observed to have an intense maximum at an angle of 20° from the incident direction. Assuming $n = 1$ (from the intensity), what must be the wavelength of the incident radiation?

Solution: Notice that the angle between the incident beam and scattered wave for constructive interference is always 2θ (see Figures 5.4 and 5.5). Thus $\theta = 10°$, but in order to find λ we must know d, the lattice spacing. In Section 4.1 we showed that

$$\frac{\text{Number of molecules}}{\text{Volume}} = \frac{N_A \rho}{M}$$

where N_A is Avogadro's number, ρ is the density, and M is the gram-molecular weight. For NaCl, $\rho = 2.16 \text{ g/cm}^3$ and $M = 58.5 \text{ g/mole}$.

$$\frac{N_A \rho}{M} = \frac{\left(6.02 \times 10^{23} \dfrac{\text{molecules}}{\text{mole}}\right)\left(2.16 \dfrac{\text{g}}{\text{cm}^3}\right)}{58.5 \dfrac{\text{g}}{\text{mole}}}$$

$$= 2.22 \times 10^{22} \frac{\text{molecules}}{\text{cm}^3} = 4.45 \times 10^{22} \frac{\text{atoms}}{\text{cm}^3}$$

$$= 4.45 \times 10^{28} \frac{\text{atoms}}{\text{m}^3}$$

Because NaCl has a cubic array, we take d as the distance between Na and Cl atoms, so we have a volume of d^3 per atom.

$$\frac{1}{d^3} = 4.45 \times 10^{28} \frac{\text{atoms}}{\text{m}^3}$$

$$d = 2.82 \times 10^{-10} \text{ m} = 0.282 \text{ nm}$$

This technique of calculating the lattice spacing only works for a few cases because of the variety of crystal structures.
  We use Equation (5.1) to find λ.

$$\lambda = \frac{2d \sin \theta}{n} = \frac{(2)(0.282 \text{ nm})(\sin 10°)}{1} = 0.098 \text{ nm}$$

which is a typical x-ray wavelength. NaCl is a useful crystal for determining x-ray wavelengths and for calibrating experimental apparatus.

5.2 De Broglie Waves

By 1920 many physicists believed that a new, more general theory was needed to replace the rudimentary Bohr model of the atom. An essential step in this development was made by a young French graduate student, Prince Louis V. de Broglie (1892–1987), who began studying the problems of the Bohr model in 1920.
  De Broglie was well versed in the work of Planck, Einstein, and Bohr. He was aware of the duality of nature expressed by Einstein in which matter and energy were not independent but were in fact interchangeable. De Broglie was

After serving in World War I, Prince Louis de Broglie resumed his studies towards his doctoral degree at the University of Paris in 1924, where he reported his concept of matter waves as part of his doctoral dissertation. De Broglie spent his life in France where he enjoyed much success as an author and teacher. *AIP/Niels Bohr Library, W. F. Meggers Collection.*

particularly struck by the fact that photons (electromagnetic radiation) had both wave and corpuscular (particlelike) properties. The concept of waves is needed to understand interference and diffraction, but localized corpuscles are needed to explain phenomena like the photoelectric effect and Compton scattering. If **Wave properties of matter?** electromagnetic radiation must have *both wave and particle properties*, then why should material particles not have both wave and particle properties as well? The symmetry of nature encourages such an idea, according to de Broglie, and no laws of physics prohibit it.

When de Broglie presented his new hypothesis in a doctoral thesis to the University of Paris in 1924, it aroused considerable interest. De Broglie used Einstein's special theory of relativity together with Planck's quantum theory to establish the wave properties of particles. His fundamental relationship is the prediction that

De Broglie wavelength of a particle

$$\lambda = \frac{h}{p} \tag{5.2}$$

That is, the wavelength to be associated with a particle is given by Planck's constant divided by the particle's momentum. De Broglie was guided by the concepts of phase and group velocities of waves (see Section 5.4) to arrive at Equation (5.2). Recall that for a photon

$$E = pc$$

but $E = h\nu$, so that

$$h\nu = pc = p\lambda\nu$$

$$h = p\lambda$$

and

$$\lambda = \frac{h}{p} \tag{5.3}$$

De Broglie extended this relation for photons to all particles. Particle waves **Matter waves** were called **matter waves** by de Broglie, and the wavelength expressed in Equation (5.2) is now called the **de Broglie wavelength** of a particle.

Example 5.2

Calculate the de Broglie wavelength of (a) a tennis ball of mass 70 g traveling 25 m/s (about 56 mph) and (b) an electron of energy 50 eV.

Solution: (a) For the tennis ball, $m = 0.07$ kg, so

$$\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34} \text{ J} \cdot \text{s}}{(0.07 \text{ kg})(25 \text{ m/s})} = 3.8 \times 10^{-34} \text{ m}$$

(b) For the electron, it is more convenient to use eV units, so we rewrite the wavelength λ as

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mK}} = \frac{hc}{\sqrt{2(mc^2)K}}$$

$$\lambda = \frac{1240 \text{ eV} \cdot \text{nm}}{\sqrt{2(0.511 \times 10^6 \text{ eV})(50 \text{ eV})}} = 0.17 \text{ nm}$$

Note that because the kinetic energy of the electron is so small, we have used the nonrelativistic calculation. Calculations in modern physics are normally done using eV units, both because it is easier and also because eV values are more appropriate for atoms and nuclei (MeV, GeV) than are joules. The values of hc and some masses can be found inside the front cover.

How can we show whether such objects as the tennis ball or the electron in the previous example exhibit wavelike properties? The best way is to pass the objects through a slit having a width of the same dimension as the object's wavelength. We expect it to be very difficult to demonstrate interference or diffraction for the tennis ball, even if we could find a slit as narrow as 10^{-34} m (which we can't!). It is unlikely we will ever be able to demonstrate the wave properties of the tennis ball. But the de Broglie wavelength of the electron, in this case ~0.2 nm, is large enough that we should be able to demonstrate its wave properties. Because of their small mass, electrons can have a small momentum and in turn a large wavelength ($\lambda = h/p$). Electrons offer perhaps our best chance of observing effects due to matter waves.

FIGURE 5.7 A schematic diagram of waves in an electron orbit around a nucleus. An integral number of wavelengths fits in the orbit. Note that the electron does not "wiggle" around the nucleus. The displacement from the dashed line represents an amplitude.

Bohr's Quantization Condition

One of Bohr's assumptions concerning his hydrogen atom model was that the angular momentum of the electron-nucleus system in a stationary state is an integral multiple of $h/2\pi$. Let's now see if we can predict this result using de Broglie's result. Represent the electron as a standing wave in an orbit around the proton. This standing wave will have nodes and be an integral number of wavelengths. We show an example of this in Figure 5.7. In order for it to be a correct standing wave, we must have

$$n\lambda = 2\pi r$$

where r is the radius of the orbit. Now we use the de Broglie relation for the wavelength and obtain

$$2\pi r = n\lambda = n\frac{h}{p}$$

The angular momentum of the electron in this orbit is $L = rp$, so we have, using the above relation,

$$L = rp = \frac{nh}{2\pi} = n\hbar$$

We have arrived at Bohr's quantization assumption by simply applying de Broglie's wavelength for an electron in a standing wave. This result hardly seems fortuitous, but though firm experimental proof was still lacking, it was soon to come.

5.3 Electron Scattering

In 1925 C. Davisson and L. H. Germer worked at Bell Telephone Laboratories investigating the properties of metallic surfaces by scattering electrons from various materials when a liquid air bottle exploded near their apparatus. Because the nickel target they were currently bombarding was at a high temperature when the accident occurred, the subsequent breakage of their vacuum system caused significant oxidation of the nickel. The target had been specially prepared and was rather expensive, so they tried to repair it by, among other procedures, prolonged heating at various high temperatures in hydrogen and under vacuum to deoxidize it.
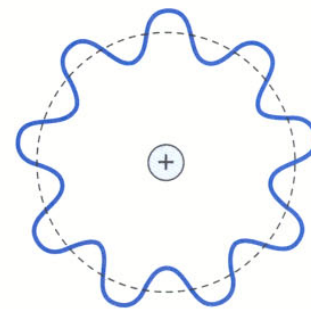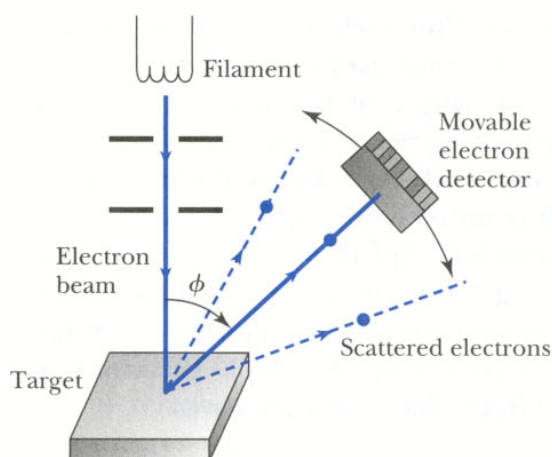
FIGURE 5.8 Schematic diagram of Davisson-Germer experiment. Electrons are produced by the hot filament, accelerated, and focused onto the target. Electrons are scattered at an angle ϕ into a detector, which is movable. The distribution of electrons is measured as a function of ϕ. The entire apparatus is located in a vacuum.

A simple diagram of the Davisson-Germer apparatus is shown in Figure 5.8. Upon putting the refurbished target back in place and continuing the experiments, Davisson and Germer found a striking change in the way electrons were scattering from the nickel surface. They had previously seen a smooth variation of intensity with scattering angle, but the new data showed large increases for certain energies at a given scattering angle. Davisson and Germer were so puzzled by their new data, that after a few days, they cut open the tube in order to examine the nickel target. They found that the polycrystalline structure of the nickel had been modified by the high temperature. The many small crystals of the original target had been changed into a few large crystals as a result of the heat treatment. Davisson surmised it was this new crystal structure of nickel—the arrangement of atoms in the crystals, not the structure of the atoms—that had caused the new intensity distributions. Some 1928 experimental results of Davisson and Germer for 54-eV electrons scattered from nickel are shown in Figure 5.9. The scattered peak occurs for $\phi = 50°$.

A lucky accident?

Diffraction of electrons

The electrons were apparently being diffracted much like x rays, and Davisson, being aware of de Broglie's results, found that the Bragg law applied to their data as well. Davisson and Germer were able to vary the scattering angles for a given wavelength and vary the wavelength (by changing the electron accelerating voltage and thus the momentum) for a given angle.
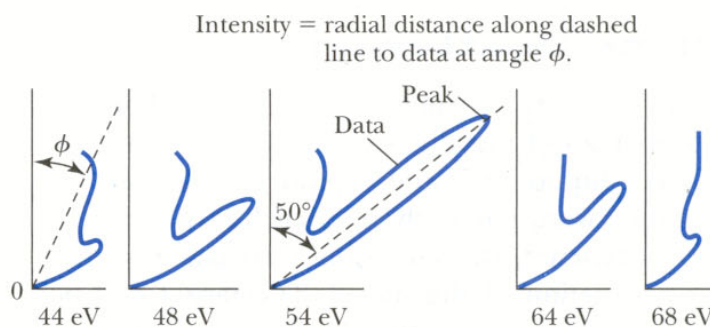

FIGURE 5.9 Davisson and Germer data for scattering of electrons from Ni. The peak $\phi = 50°$ builds dramatically as the energy of the electron nears 54 eV. *From C. J. Davisson, Journal of The Franklin Institute **205**, 597–623 (1928).*
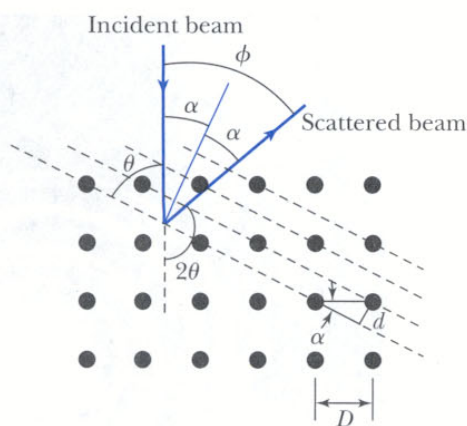
FIGURE 5.10 The scattering of electrons by lattice planes in a crystal. This figure is useful to compare the scattering relations $n\lambda = 2d \sin \theta$ and $n\lambda = D \sin \phi$ where θ and ϕ are angles shown, D = interatomic spacing, and d = lattice plane spacing.

The relationship between the incident electron beam and the nickel crystal is shown in Figure 5.10. In the Bragg Law, 2θ is the angle between the incident and exit beams. Therefore, $\phi = \pi - 2\theta = 2\alpha$. Because $\sin \theta = \cos(\phi/2) = \cos \alpha$, we have for the Bragg condition, $n\lambda = 2d \cos \alpha$. However, d is the lattice plane spacing and is related to the interatomic distance D by $d = D \sin \alpha$ so that

$$n\lambda = 2d \sin \theta = 2d \cos \alpha = 2D \sin \alpha \cos \alpha$$

$$n\lambda = D \sin 2\alpha = D \sin \phi \tag{5.4}$$

or

$$\lambda = \frac{D \sin \phi}{n} \tag{5.5}$$

For nickel the interatomic distance is $D = 0.215$ nm. If the peak found by Davisson and Germer at 50° was $n = 1$, then the electron wavelength should be

$$\lambda = (0.215 \text{ nm})(\sin 50°) = 0.165 \text{ nm}$$

Let us now compare this wavelength with that expected for a 54-eV electron. We can determine the electron's momentum nonrelativistically from the kinetic energy.

$$\frac{p^2}{2m} = \text{K.E.} = eV_0 \tag{5.6}$$

where V_0 is the voltage through which the electrons are accelerated. We find the momentum to be $p = \sqrt{(2m)(eV_0)}$. The de Broglie wavelength is now

$$\lambda = \frac{h}{p} = \frac{hc}{pc} = \frac{hc}{\sqrt{(2mc^2)(eV_0)}} = \frac{1240 \text{ eV} \cdot \text{nm}}{\sqrt{(2)(0.511 \times 10^6 \text{ eV})(eV_0)}} \tag{5.7}$$

$$= \frac{1.226 \text{ nm} \cdot \text{V}^{1/2}}{\sqrt{V_0}}$$

where the constants h, c, and m have been evaluated and V_0 is the voltage. For $V_0 = 54$ V, the wavelength is

$$\lambda = \frac{1.226 \text{ nm} \cdot \text{V}^{1/2}}{\sqrt{54 \text{ V}}} = 0.167 \text{ nm}$$

Clinton J. Davisson (1881–1958) is shown here in 1928 on the right looking at the electronic diffraction tube held by Lester H. Germer (1896–1971). They performed their work at Bell Telephone Laboratory. Davisson received the Nobel Prize in physics in 1937. *AIP Emilio Segrè Visual Archives.*
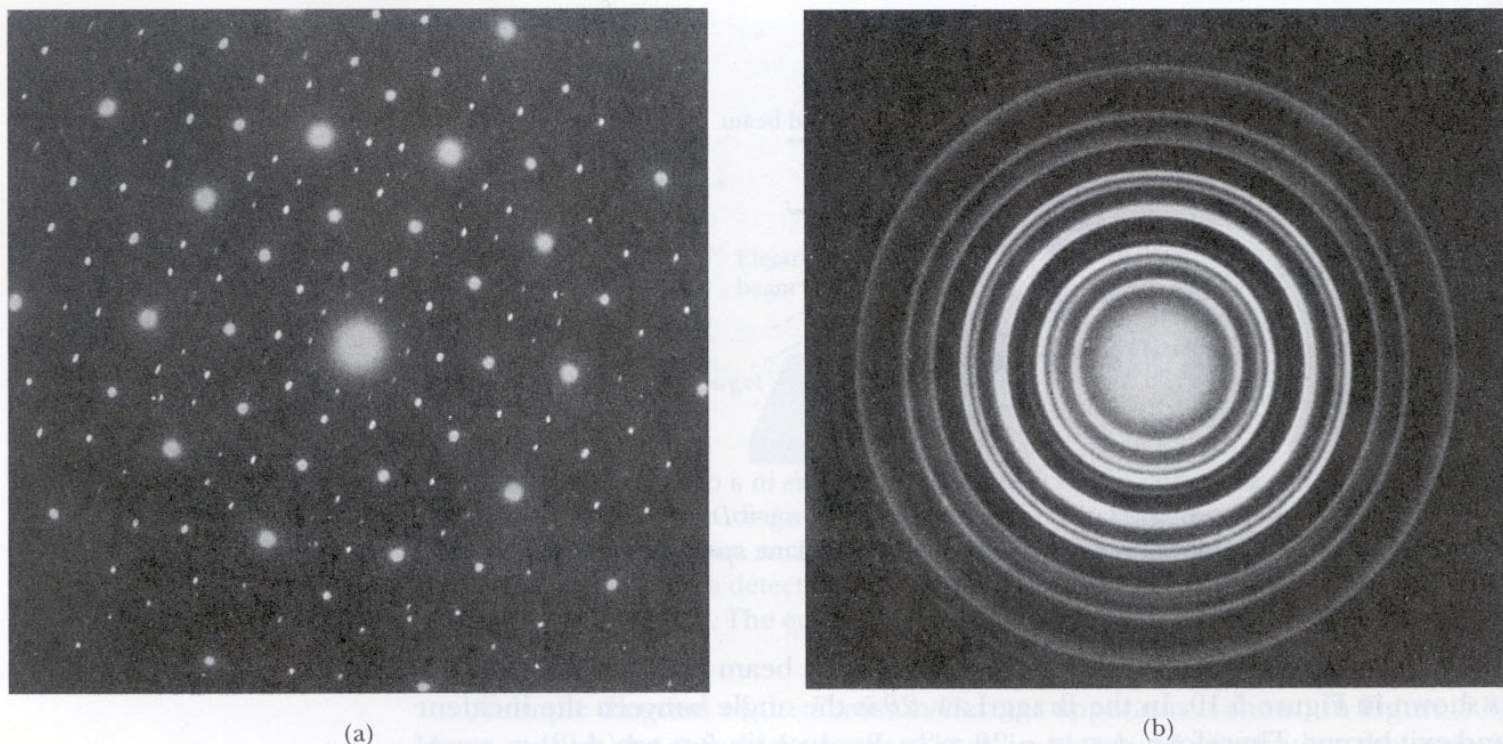
(a)

(b)

FIGURE 5.11   Examples of transmission electron diffraction photographs. (a) Produced by scattering 120-keV electrons on the quasicrystal $Al_{80}Mn_{20}$. (b) An early pattern from polycrystalline SnO_2. Notice that the dots in (a) indicate that the sample was a crystal whereas the rings in (b) indicate that a randomly oriented sample (or powder) was used. *(a) is courtesy of David Follstaedt, Sandia National Laboratory. (b) is from G. P. Thomson and W. Cochrane, Theory and Practice of Electron Diffraction. London: Macmillan, 1939.*

This value of the wavelength is in good agreement with that found earlier for the peak at 50°.

Shortly after Davisson and Germer reported their experiment, George P. Thomson (1892–1975), son of J. J. Thomson, reported seeing the effects of electron diffraction in transmission experiments. The first target was celluloid, and soon after that gold, aluminum, and platinum were used. Beautiful rings are obtained, as is shown for SnO_2 in Figure 5.11. Davisson and Thomson received the Nobel Prize in 1937 for their investigations, which clearly showed that particles exhibited wave properties. In the next few years hydrogen and helium atoms were also shown to exhibit wave diffraction. An important modern measurement technique uses diffraction of neutrons to study the crystal and molecular structure of biologically important substances. All these experiments are consistent with the de Broglie hypothesis for the wavelength of a massive particle.

Example 5.3

In introductory physics, we learned that a particle (ideal gas) in thermal equilibrium with its surroundings has a kinetic energy of $3kT/2$. Calculate the de Broglie wavelength for (a) a neutron at room temperature (300 K) and (b) a "cold" neutron at 77 K (liquid nitrogen).

Solution: We begin by finding the de Broglie wavelength of the neutron from the momentum.

$$\frac{p^2}{2m} = \text{K.E.} = \frac{3}{2}kT \qquad (5.8)$$

$$p = \sqrt{3mkT}$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{3mkT}} = \frac{hc}{\sqrt{3(mc^2)kT}}$$

$$= \frac{1}{T^{1/2}} \frac{1240 \text{ eV} \cdot \text{nm}}{\sqrt{3(938 \times 10^6 \text{ eV})(8.62 \times 10^{-5} \text{ eV/K})}}$$

It again has been convenient to use eV units.

$$\lambda = \frac{2.52}{T^{1/2}} \text{ nm} \cdot \text{K}^{1/2} \qquad (5.9)$$

$$\lambda(300 \text{ K}) = \frac{2.52 \text{ nm} \cdot \text{K}^{1/2}}{\sqrt{300 \text{ K}}} = 0.145 \text{ nm} \qquad (5.9a)$$

$$\lambda(77 \text{ K}) = \frac{2.52 \text{ nm} \cdot \text{K}^{1/2}}{\sqrt{77 \text{ K}}} = 0.287 \text{ nm} \qquad (5.9b)$$

These wavelengths are thus suitable for diffraction by crystals. "Supercold" neutrons, used to produce even larger wavelengths, are useful because extraneous electric and magnetic fields do not affect neutrons as much as electrons.

5.4 Wave Motion

Because particles exhibit wave behavior, it must be possible to formulate a wave description of particle motion. Our development of quantum theory will be based heavily on waves, so now we digress briefly to review the elementary physics of wave motion, which we shall ultimately apply to particles.

In elementary physics, we study waves of several kinds, including sound waves and electromagnetic waves (including light). The simplest form of wave has a sinusoidal form; at a fixed time (say, $t = 0$) its spatial variation looks like

$$\Psi(x, t)\Big|_{t=0} = A \sin\left(\frac{2\pi}{\lambda} x\right) \qquad (5.10)$$

as is shown in Figure 5.12. The function $\Psi(x, t)$ represents the *instantaneous amplitude* or *displacement* of the wave as a function of position x and time t. In the case of a wave moving down a string, Ψ is the displacement of the string; in the case of a sound wave, Ψ is the displacement of the air molecules; and in the case of electromagnetic radiation, Ψ is the electric field **E** or magnetic field **B**. The maximum displacement A is normally called the **amplitude,** but a better term for a harmonic wave such as we are considering may be **harmonic amplitude.**

As time increases the position of the wave will change, so the general expression for the wave is

$$\Psi(x, t) = A \sin\left[\frac{2\pi}{\lambda}(x - vt)\right] \qquad (5.11) \qquad \textbf{Wave form}$$

The position at time $t = t_0$ is also shown in Figure 5.12. The **wavelength** λ is defined to be the distance between points in the wave with the same phase, for example, positive wave crests. The **period** T is the time required for a wave to travel a distance of one wavelength λ. Because the velocity [actually phase velocity, see Equation (5.17)] of the wave is v, we have $\lambda = vT$. The frequency $\nu(= 1/T)$ of a

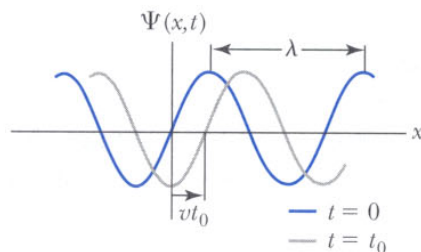**Wavelength**

Period

FIGURE 5.12 Wave form of a wave moving to the right at speed v shown at $t = 0$ and $t = t_0$.

harmonic wave is the number of times a crest passes a given point (a complete *cycle*) per second. A traveling wave of the type described by Equation (5.11) satisfies the wave equation,*

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 \Psi}{\partial t^2} \tag{5.12}$$

If we use $\lambda = vT$, we can rewrite Equation (5.11).

$$\Psi(x, t) = A \sin\left[2\pi\left(\frac{x}{\lambda} - \frac{t}{T}\right)\right] \tag{5.13}$$

Wave number and angular frequency   We can write Equation (5.13) more compactly by defining the **wave number** k and **angular frequency** ω by

$$k \equiv \frac{2\pi}{\lambda} \quad \text{and} \quad \omega \equiv \frac{2\pi}{T} \tag{5.14}$$

Equation (5.13) then becomes

$$\Psi(x, t) = A \sin(kx - \omega t) \tag{5.15}$$

This is the mathematical description of a sine curve traveling in the positive x direction that has a displacement $\Psi = 0$ at $x = 0$ and $t = 0$. A similar wave traveling in the negative x direction would have the form

$$\Psi(x, t) = A \sin(kx + \omega t) \tag{5.16}$$

The **phase velocity** v_{ph} is the velocity of a point on the wave that has a given phase (for example, the crest) and is given by

Phase velocity

$$v_{\text{ph}} = \frac{\lambda}{T} = \frac{\omega}{k} \tag{5.17}$$

If the wave does not have $\Psi = 0$ at $x = 0$ and $t = 0$, we can describe the wave using a **phase constant** ϕ

$$\Psi(x, t) = A \sin(kx - \omega t + \phi) \tag{5.18}$$

For example, if $\phi = 90°$, Equation (5.18) can be written

$$\Psi(x, t) = A \cos(kx - \omega t) \tag{5.19}$$

Observation of many different kinds of waves has established the general result that when two or more waves traverse the same region, they act independently of each other. According to the **principle of superposition,** we add the displacements of all waves present. A familiar example is the superposition of two sound waves of nearly equal frequencies: The phenomenon of beats is observed. Examples of superposition are shown in Figure 5.13. The net displacement depends on the harmonic amplitude, the phase, and the frequency of each of the individual waves.

Principle of superposition

How might we use waves to represent a moving particle? In Figure 5.13 we see that when two waves are added together, we obtain regions of relatively large (and small) displacement. If we add many waves of different amplitudes and frequencies in particular ways, it is possible to obtain what is called a **wave packet.** The important property of the wave packet is that its net amplitude differs from

Wave packet

*The derivation of the wave equation is presented in most introductory physics textbooks for a wave on a string, although it is often an optional section and skipped. It would be worthwhile for the student to review its derivation now, especially the use of the partial derivatives.
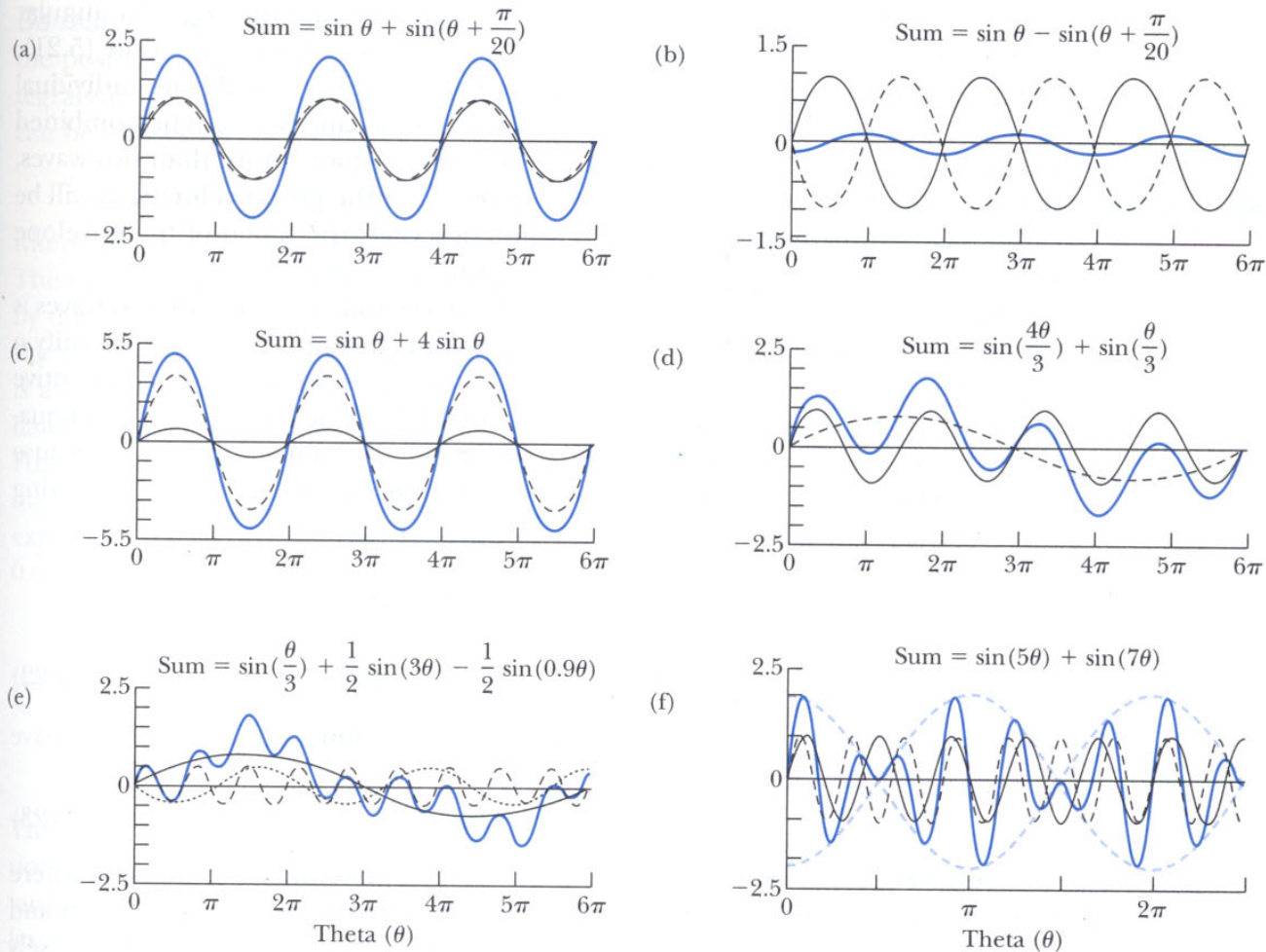
(a) Sum $= \sin\theta + \sin(\theta + \frac{\pi}{20})$

(b) Sum $= \sin\theta - \sin(\theta + \frac{\pi}{20})$

(c) Sum $= \sin\theta + 4\sin\theta$

(d) Sum $= \sin(\frac{4\theta}{3}) + \sin(\frac{\theta}{3})$

(e) Sum $= \sin(\frac{\theta}{3}) + \frac{1}{2}\sin(3\theta) - \frac{1}{2}\sin(0.9\theta)$

(f) Sum $= \sin(5\theta) + \sin(7\theta)$

Theta (θ) Theta (θ)

FIGURE 5.13 Superposition of waves. The heavy blue line is the resulting wave. (a) Two waves of equal frequency and amplitude that are almost in phase. The result is a larger wave. (b) As in (a) but the two waves are almost out of phase. The result is a smaller wave. (c) Superposition of two waves with the same frequency, but different amplitudes. (d) Superposition of two waves of equal amplitude but different frequencies. (e) Superposition of three waves of different amplitudes and frequencies. (f) Superposition of two waves of almost the same frequency over many wavelengths, indicating the phenomenon of beats.

zero only over a small region Δx as shown in Figure 5.14. We can localize the position of a particle in a particular region by using a wave packet description.

Let us examine in detail the superposition of two waves. Assume both waves have the same harmonic amplitude A but different wave numbers (k_1 and k_2) and angular frequencies (ω_1 and ω_2). The superposition of the two waves is the sum

$$\Psi(x, t) = \Psi_1(x, t) + \Psi_2(x, t) = A\cos(k_1 x - \omega_1 t) + A\cos(k_2 x - \omega_2 t) \quad (5.20)$$

$$= 2A\cos\left[\frac{1}{2}(k_1 - k_2)x - \frac{1}{2}(\omega_1 - \omega_2)t\right]\cos\left[\frac{1}{2}(k_1 + k_2)x - \frac{1}{2}(\omega_1 + \omega_2)t\right]$$

$$= 2A\cos\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)\cos(k_{av}x - \omega_{av}t) \quad (5.21)$$

where $\Delta k = k_1 - k_2$, $\Delta\omega = \omega_1 - \omega_2$, $k_{av} = (k_1 + k_2)/2$, and $\omega_{av} = (\omega_1 + \omega_2)/2$. We exhibited similar waves in Figure 5.13a–d, where the heavy solid line indicates the resulting wave. In Figure 5.13f the blue dashed line indicates an envelope which denotes the maximum displacement of the combined waves. The
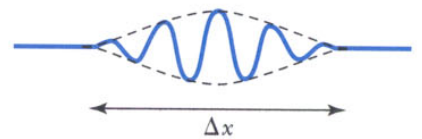

FIGURE 5.14 An idealized wave packet localized in space over a region Δx is the superposition of many waves of different amplitudes and frequencies.

wave still oscillates within this envelope with the wave number k_{av} and angular frequency ω_{av}. The envelope is described by the first term of Equation (5.21), which has the wave number $\Delta k/2$ and angular frequency $\Delta\omega/2$. The individual waves each move with their own phase velocity: ω_1/k_1 and ω_2/k_2. The combined wave has a phase velocity ω_{av}/k_{av}. When combining many more than two waves, one obtains a pulse, or wave packet, which moves at the **group velocity,** as will be shown later. Only the group velocity, which describes the speed of the envelope ($u_{gr} = \Delta\omega/\Delta k$), is important when dealing with wave packets.

Phase and group velocities

In contrast to the pulse or wave packet, the combination of only two waves is not localized in space. However, for purposes of illustration, we can identify a "localized region" $\Delta x = x_2 - x_1$ where x_1 and x_2 represent two consecutive points where the envelope is zero (see Figure 5.13f). The term $\Delta k \cdot x/2$ in Equation (5.21) must be different by a phase of π for the values x_1 and x_2, because $x_2 - x_1$ represents only one half of the wavelength of the envelope confining the wave.

$$\frac{1}{2} \Delta k \, x_2 - \frac{1}{2} \Delta k \, x_1 = \pi$$

$$\Delta k(x_2 - x_1) = \Delta k \, \Delta x = 2\pi \tag{5.22}$$

Similarly, for a given value of x we can determine the time Δt over which the wave is localized and obtain

$$\Delta\omega \, \Delta t = 2\pi \tag{5.23}$$

The results of Equations (5.22) and (5.23) can be generalized to the case where there are many waves forming the wave packet. The equations, $\Delta k \, \Delta x = 2\pi$ and $\Delta\omega \, \Delta t = 2\pi$, are significant because they tell us that in order to know precisely the position of the wave packet envelope (Δx small), we must have a large range of wave numbers (Δk large). Similarly, to know precisely when the wave is at a given point (Δt small), we must have a large range of frequencies ($\Delta\omega$ large). Equation (5.23) is the origin of the bandwidth relation important in electronics. A particular circuit component must have a large bandwidth $\Delta\omega$ in order for its signal to respond in a short time (Δt).

If we are to treat particles as matter waves, we have to be able to describe the particle in terms of waves. An important aspect of a particle is its localizing in space. That is why it is so important to form the wave packet that we have been discussing. We extend Equation (5.20) by summing over many waves with possibly different wave numbers, angular frequencies, and amplitudes.

$$\Psi(x, t) = \sum_i A_i \cos(k_i x - \omega_i t) \tag{5.24}$$

Fourier series and integral

Such a result is called a **Fourier series.** When dealing with a continuous spectrum, it may be desirable to extend Equation (5.24) to the integral form called a **Fourier integral.**

$$\Psi(x, t) = \int \widetilde{A}(k) \cos(kx - \omega t) \, dk \tag{5.25}$$

The amplitudes A_i and $\widetilde{A}(k)$ may be functions of k. The use of Fourier series and Fourier integrals is at a more advanced level of mathematics than we want to pursue now.* We can, however, indicate their value by one important example.

*See John D. McGervey, *Introduction to Modern Physics*, Chap. 4. Orlando, FL: Academic Press, 1983.

Gaussian Wave Packet. Gaussian wave packets are often used to represent the position of particles, as illustrated in Figure 5.15, because the associated integrals are relatively easy to evaluate. At a given time t, say $t = 0$, a Gaussian wave can be expressed as

$$\Psi(x, 0) = \psi(x) = Ae^{-\Delta k^2 x^2} \cos(k_0 x) \qquad (5.26)$$

Gaussian function

where Δk expresses the range of wave numbers used to form the wave packet. The $\cos(k_0 x)$ term describes the wave oscillating inside the envelope described by the (Gaussian) exponential term $e^{-\Delta k^2 x^2}$. The intensity distribution $\mathcal{I}(k)$ for the wave numbers leading to Equation (5.26) is shown in Figure 5.15a. There is a high probability of a particular measurement of k being within one standard deviation of the mean value k_0. The function $\psi(x)$ is shown in Fig. 5.15b. For simplicity, let the constant A be one. There is a good probability of finding the particle within the values of $x = 0$ ($\psi(x) = 1$) and $x = \Delta x/2$ ($\psi(x) = \exp(-\Delta k^2 \Delta x^2/4)$). Roughly, the value of $\psi(x)$ at the position $x = \Delta x/2$ is about 0.6 (see Figure 5.15b), so we have

$$e^{-\Delta k^2 \Delta x^2/4} \approx 0.6$$

We take the logarithm of both sides and find

$$-\frac{\Delta k^2 \Delta x^2}{4} \approx -0.5 \qquad \text{or} \qquad \Delta k \, \Delta x \approx 1.4 \qquad (5.27)$$

This has been a very rough calculation, and the answer depends on the assumptions we have made. A more detailed calculation gives $\Delta k \, \Delta x = 1/2$. The important point is that with the Gaussian wave packet, we have arrived at a result similar to Equation (5.22), namely, that the product $\Delta k \, \Delta x$ is about unity. The localization of the wave packet over a small region Δx to describe a particle requires a large range of wave numbers; that is, Δk is large. Conversely, a small range of wave numbers cannot produce a wave packet localized within a small distance.
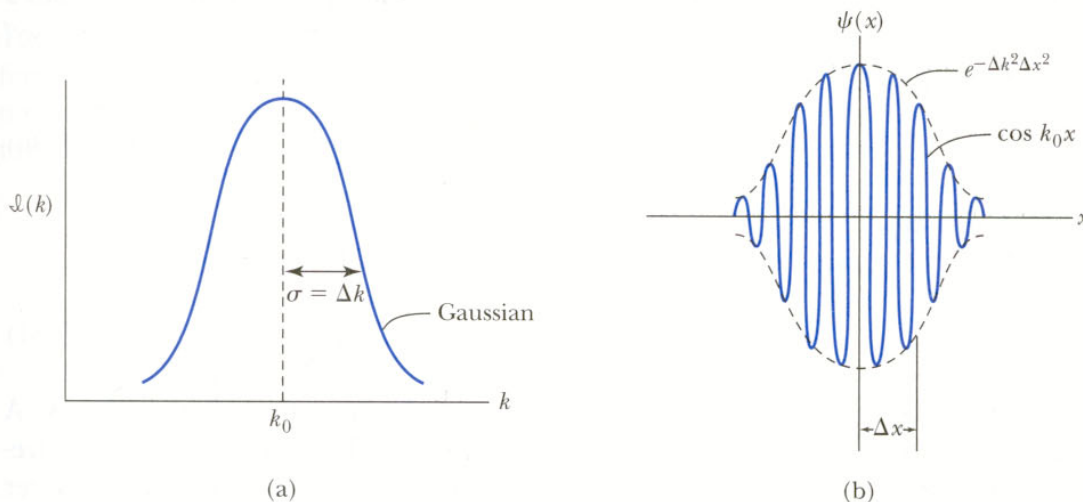
FIGURE 5.15 The form of the probability distribution or intensity $\mathcal{I}(k)$ shown in (a) is taken to have a Gaussian shape with a standard deviation of Δk (determined when the function $\exp[-(k - k_0)^2/2\sigma^2]$ has $k = k_0 \pm \Delta k$ and $\Delta k = \sigma$, the standard deviation). This $\mathcal{I}(k)$ leads to $\psi(x)$, as is shown in (b). The envelope for $\psi(x)$ is described by the $\exp(-\Delta k^2 x^2)$ term with the oscillating term $\cos(k_0 x)$ contained by the envelope. At the given time $t = 0$, the wave packet (particle) is localized to the area $x \approx 0 \pm \Delta x$ with wave numbers $k \approx k_0 \pm \Delta k$.

To complete our study of waves and the representation of particles by wave packets, we must be convinced that the superposition of waves is actually able to describe particles. We found earlier for the superposition of two waves that the group velocity, $u_{gr} = \Delta\omega/\Delta k$, represented the motion of the envelope. We can generalize this for the case of the wave packet and will find that the wave packet moves with the group velocity u_{gr} given by

Group velocity

$$u_{gr} = \frac{d\omega}{dk} \tag{5.28}$$

Because the wave packet consists of many wave numbers, we should remember to evaluate this derivative at the center of the wave packet (that is, $k = k_0$).

For a de Broglie wave, we have $E = h\nu$ and $p = h/\lambda$. We can rewrite both of these equations in terms of $\hbar$.

$$E = h\nu = \hbar(2\pi\nu) = \hbar\omega$$

$$p = \frac{h}{\lambda} = \hbar\frac{2\pi}{\lambda} = \hbar k$$

where we have used the relations $\omega = 2\pi\nu$ and $k = 2\pi/\lambda$. If we multiply the denominator and numerator in Equation (5.28) by $\hbar$, we have

$$u_{gr} = \frac{d\omega}{dk} = \frac{d(\hbar\omega)}{d(\hbar k)} = \frac{dE}{dp}$$

We use the relativistic relation $E^2 = p^2c^2 + m^2c^4$ and the derivative of E to find

$$2E\,dE = 2pc^2\,dp$$

or

$$u_{gr} = \frac{dE}{dp} = \frac{pc^2}{E} \tag{5.29}$$

This is the velocity of a particle of momentum p and total energy E. Thus, it is plausible to assume that the group velocity of the wave packet can be associated with the velocity of a particle.

The phase velocity of a wave is represented by

$$v_{ph} = \lambda\nu = \frac{\omega}{k} \tag{5.30}$$

so that $\omega = kv_{ph}$.

Then, the group velocity is related to the phase velocity by

$$u_{gr} = \frac{d\omega}{dk} = \frac{d}{dk}(v_{ph}k) = v_{ph} + k\frac{dv_{ph}}{dk} \tag{5.31}$$

Thus, the group velocity may be greater or less than the phase velocity. A medium is called *nondispersive* when the phase velocity is the same for all frequencies and $u_{gr} = v_{ph}$. An example is electromagnetic waves in vacuum. Water waves are a good example of waves in a dispersive medium. When one throws a rock in a still pond, the envelope of the waves moves more slowly than the individual waves moving outward (see Figure 5.16).

Dispersion plays an important role in the shape of wave packets. For example, in the case of the Gaussian wave packet shown in Figure 5.15 at $t = 0$, the wave packet will spread out as time progresses. A packet that is highly localized at one time will have its waves added together in a considerably different manner at another time due to the superposition of the waves.
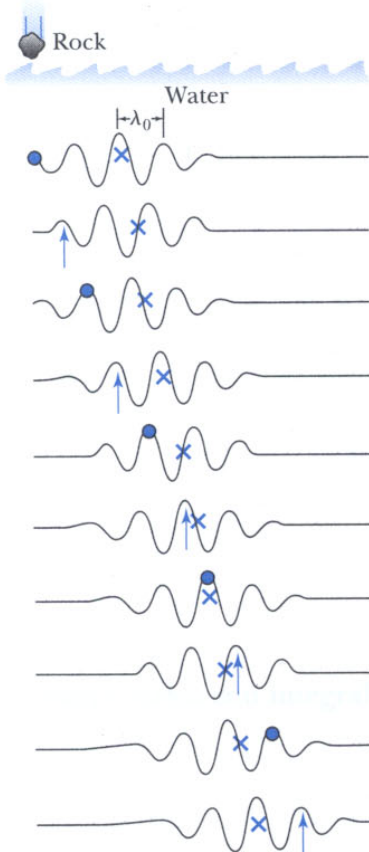

FIGURE 5.16 Progression with time of wave packet for which $u_{gr} = v_{ph}/2$. Note how the individual wave (arrow and dot alternate) moves through the wave packet (letter ✕) with time.

Example 5.4

Newton showed that deep-water waves have a phase velocity of $\sqrt{g\lambda/2\pi}$. Find the group velocity of such waves and discuss the motion.

Solution: We use Equation (5.31) to relate the group and phase velocities, but first we need to write the phase velocity v_{ph} in terms of k. If we use $\lambda = 2\pi/k$, we have

$$v_{ph} = \sqrt{\frac{g\lambda}{2\pi}} = \sqrt{\frac{g}{k}} = \sqrt{g}\,k^{-1/2}$$

Now we can take the necessary derivative for Equation (5.31).

$$u_{gr} = \sqrt{\frac{g}{k}} + k\frac{d}{dk}\left[\sqrt{g}\,k^{-1/2}\right] = \sqrt{\frac{g}{k}} + k\sqrt{g}\left[-\frac{1}{2}k^{-3/2}\right]$$

$$= \sqrt{\frac{g}{k}} - \frac{1}{2}\sqrt{\frac{g}{k}} = \frac{1}{2}\sqrt{\frac{g}{k}} = \frac{1}{2}v_{ph}$$

The group velocity is determined to be one half of the phase velocity. Such an effect can be observed by throwing a rock in a still pond. As the radial waves move out, the individual waves seem to run right through the wave crests and then disappear (see Figure 5.16).

5.5 Waves or Particles?

By this point it is not unusual to be a little confused. We have been led to believe that electromagnetic radiation behaves sometimes as waves (interference and diffraction) and other times as particles (photoelectric and Compton effects). We have been presented evidence in this chapter that particles also behave as waves (electron diffraction). Can all this really be true? If a particle is a wave, what is waving? In the preceding section we learned that, at least mathematically, we could describe particles by using wave packets. Can we represent matter as waves and particles simultaneously? And can we represent electromagnetic radiation as waves and particles simultaneously? We must answer these questions of the **wave–particle duality** before proceeding with our study of quantum theory.

Wave–particle duality

Young's Double-Slit Experiment with Light. To better understand the differences and similarities of waves and particles, we analyze Young's double-slit diffraction experiment, which is studied in detail in elementary physics courses to show the interference character of light. Figure 5.17a shows a schematic
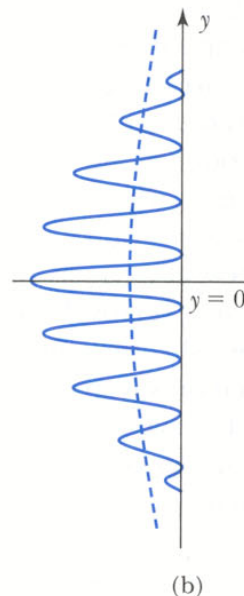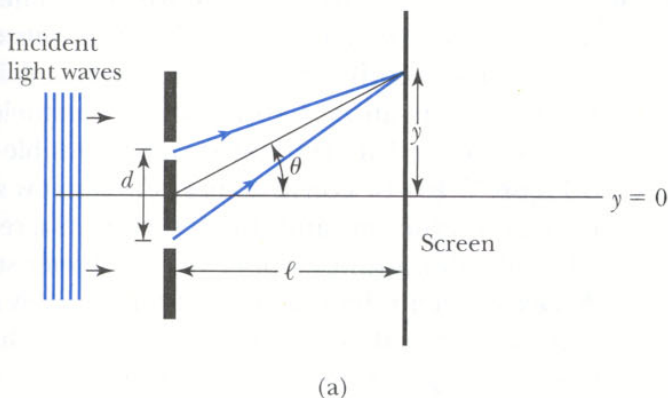

(a)

(b)

FIGURE 5.17 (a) Schematic diagram of Young's double-slit experiment. This experiment is easily performed with a laser as the light source ($\ell \gg d$, where $d =$ slit distance). (b) The solid line indicates the interference pattern due to both slits. If either of the slits is covered, single-slit diffraction gives the result shown in the dashed curve.

(a) 20 counts

(b) 100 counts

(c) 500 counts

(d) ~4000 counts

FIGURE 5.18 Computer simulation of Young's double-slit interference experiment for light or electrons. This calculation was performed for a (slit width) = 4λ, and d (slit distance) = 20λ. The four pictures are for increasing number of counts: 20, 100, 500, 4000. The interference pattern clearly has emerged for 500 counts. *Simulation and photos courtesy of Julian V. Noble.*
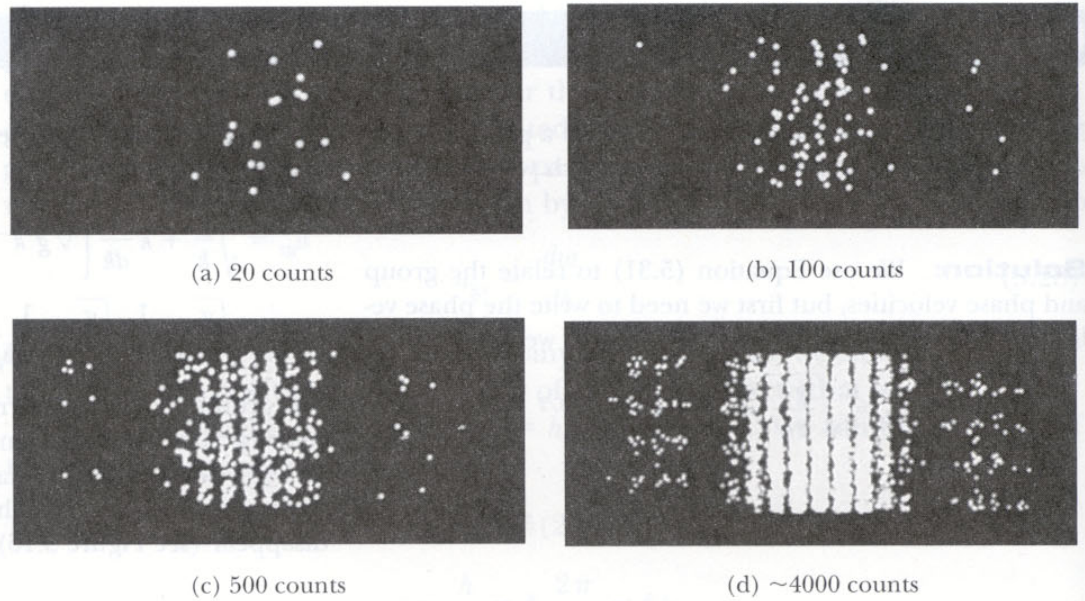
diagram of the experiment. This experiment is easily performed with the use of a low-power laser. With both slits open, a nice interference pattern is observed, with bands of maxima and minima. When one of the slits is covered, this interference pattern is changed, and a rather broad peak is observed. Thus, we conclude that the double-slit interference pattern is due to light passing through *both* slits—a wave phenomenon (see Figure 5.17b).

However, if the light intensity is reduced, and we observe the pattern on a screen, we learn that the light arriving on the screen produces flashes at various points, entirely representative of particle behavior! If we take pictures of the screen after varying lengths of time, the pictures will look like those shown in Figure 5.18. Eventually the interference pattern characteristic of wave behavior emerges. There is therefore no contradiction in this experiment. If we want to know the precise location of the light (photon), we must use the particle description and not the wave description.
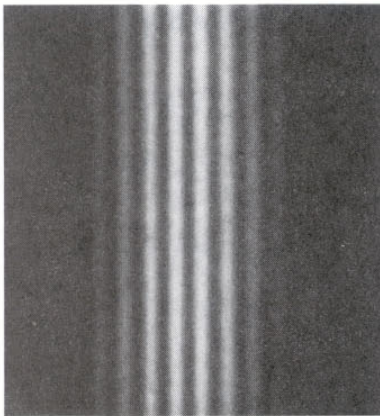
Electron Double-Slit Experiment. Now let us examine a similar double-slit experiment that uses electrons rather than light. If matter also behaves as waves, should not the same experimental results be obtained if we use electrons rather than light? The answer is yes, and physicists did not doubt the eventual result. This experiment is not as easy to perform as the similar one with light. The difficulty arises in constructing slits narrow enough to exhibit wave phenomena. This requires $\lambda \sim a$, where a is the slit width. For light of $\lambda = 600$ nm, slits can be produced mechanically. However, for electrons of energy 50 keV, $\lambda \approx 5 \times 10^{-3}$ nm, which is smaller than a hydrogen atom (~0.1 nm). Nevertheless, C. Jönsson* of Tübingen, Germany, succeeded in 1961 in showing double-slit interference effects for electrons (Figure 5.19) by constructing very narrow slits and using relatively large distances between the slits and the observation screen. Copper slits were made by electrolytically depositing copper on a polymer strip printed on silvered glass plates. This experiment demonstrated that precisely the same behavior occurs for both light (waves) and electrons (particles). We have seen similar behavior previously from the Debye-Scherrer rings produced by the diffraction of x rays (waves) and electrons (particles).

FIGURE 5.19 Demonstration of electron interference using two slits similar in concept to Young's double-slit experiment for light. This result by Claus Jönsson clearly shows that electrons exhibit wave behavior (see also Example 5.5). *Reprinted with permission from C. Jönsson, American Journal of Physics, 42, 4 (1974). © 1974 American Association of Physics.*

*C. Jönsson, *Am. J. Phys.* **42, 4** (1974), translation of *Zeitschrift f. Physik* **161**, 454 (1961).

Example 5.5

In the experiment by Jönsson, 50-keV electrons impinged on slits of width 500 nm separated by a distance of 2000 nm. The observation screen was located 350 mm beyond the slits. What was the distance between the first two maxima?

Solution: The equation specifying the orders of maxima and the angle θ from incidence is (see Figure 5.17)

$$d \sin \theta = n\lambda \qquad (5.32)$$

The order $n = 0$ has $\theta = 0$, and the next maximum, $n = 1$, is

$$\sin \theta = \frac{\lambda}{d} = \frac{\lambda}{2000 \text{ nm}}$$

We have already calculated the wavelength for electrons of energy eV_0 in Equation (5.7).

$$\lambda = \frac{1.226 \text{ nm} \cdot \text{V}^{1/2}}{\sqrt{50 \times 10^3 \text{ V}}} = 5.48 \times 10^{-3} \text{ nm}$$

Because 50 keV may be too high an energy for a nonrelativistic calculation such as that done in Equation (5.7), we had better perform a relativistic calculation to be certain. We first find the momentum and insert that into $\lambda = h/p$.

$$(pc)^2 = E^2 - E_0^2 = (K + E_0)^2 - E_0^2$$

$$= (50 \times 10^3 \text{ eV} + 0.511 \times 10^6 \text{ eV})^2 -$$

$$(0.511 \times 10^6 \text{ eV})^2 = (0.231 \times 10^6 \text{ eV})^2$$

Now we can determine the wavelength.

$$\lambda = \frac{h}{p} = \frac{hc}{pc} = \frac{1240 \text{ eV} \cdot \text{nm}}{0.231 \times 10^6 \text{ eV}} = 5.36 \times 10^{-3} \text{ nm}$$

Therefore, we find the more accurate relativistic value to be somewhat less (2%) than the nonrelativistic value. Now we can determine the angle.

$$\sin \theta = \frac{5.36 \times 10^{-3} \text{ nm}}{2000 \text{ nm}} = 2.68 \times 10^{-6}$$

The distance of the first maximum along the screen is $y = \ell \tan \theta$, but for such a small angle, $\sin \theta = \tan \theta$.

$$y = \ell \tan \theta \approx \ell \sin \theta = 350 \text{ mm}(2.68 \times 10^{-6})$$

$$= 9.38 \times 10^{-4} \text{ mm} \frac{10^6 \text{ nm}}{\text{mm}} = 938 \text{ nm}$$

Such a diffraction pattern is too small to be viewed by eye. Jönsson magnified the pattern by a series of electronic lenses and then observed a fluorescent screen with a ten-power optical microscope.

Another Gedanken Experiment. If we were to cover one of the slits in the preceding Jönsson experiment, the double-slit interference pattern would be destroyed—just as it was when light was used. But our experience tells us the electron is a particle, and we know that it can go through only one of the slits. Let's devise a *gedanken* experiment, shown in Figure 5.20, to determine which slit the electron went through. We set up a light shining on the double slit and use a powerful microscope to look at the region. After the electron passes through one of the slits, light bounces off the electron; we observe the light, so we know which slit the electron came through.
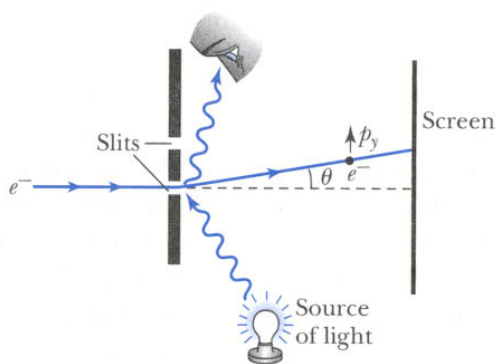
Which slit does the electron pass through?

FIGURE 5.20 An attempt to measure which slit an electron passes through in the double-slit experiment. A powerful light source scatters a photon from the electron, and the scattered photon is observed. The motion of the electron is affected.

In order to do this experiment, we need to use light having wavelength narrower than the slit separation d, in order to determine which slit the electron went through. We use a subscript ph to denote variables for light (photon). Therefore, we have $\lambda_{ph} < d$. The momentum of the photon is

$$p_{ph} = \frac{h}{\lambda_{ph}} > \frac{h}{d}$$

For us to show the interference effects for the electrons passing through the slits, the electrons must also have a wavelength on the order of the slit separation d, $\lambda_{el} \sim d$. The momentum of the electrons will be on the order of

$$p_{el} = \frac{h}{\lambda_{el}} \sim \frac{h}{d}$$

The difficulty is that the momentum of the light photons used to determine which slit the electron went through is sufficiently great to strongly modify the momentum of the electron itself, thus changing the direction of the electron! The interference pattern on the screen will be changed just by requiring us to know which slit the electron went through. We will take a closer look at this experiment in Section 5.7. In trying to determine which slit the electron went through, we are examining the particlelike behavior of the electron. When we are examining the interference pattern of the electron, we are using the wavelike behavior of the electron.

Bohr resolved this dilemma by pointing out that the particlelike and wavelike aspects of nature are *complementary*. Both are needed—they just can't be observed simultaneously.

Principle of complementarity   **Bohr's principle of complementarity:** *It is not possible to simultaneously describe physical observables in terms of both particles and waves.*

Physical observables   Physical observables are those quantities such as position, velocity, momentum, and energy that can be experimentally measured. In any given instance we must use either the particle description or the wave description. Usually the choice is clear. The interference pattern of the double-slit experiment suggests that the light (or electron) had to go through both slits, and we must use the wave description. In our description of nature, we cannot describe phenomena by displaying both particle and wave behavior at the same time.

Solution of wave–particle duality   By the use of the principle of complementarity, we can solve the *wave–particle duality* problem, which has been plaguing us. It is not unusual for students to feel uncomfortable with this solution, because it cannot be directly proven. However, as a "principle" and not a "law," the complementarity principle does seem to describe nature, and, as such, we use it. We must pay close attention to the fact that we do not use waves and particles simultaneously to describe a particular phenomenon. Experiments dictate what actually happens in nature, and we must draw up a set of rules to describe our observations. These rules naturally lead to a probability interpretation of experimental observations. If we set up a series of small detectors along the screen in the electron double-slit experiment, we can speak of the probability of the electron being detected by one of the detectors. The interference pattern can guide us in our probability determinations. But once the electron has been registered by one of the detectors, the probability of its being seen in the other detectors is zero. Matter and radiation propagation is described by wavelike behavior, but matter and radiation interact (that is, creation/annihilation or detection) as particles.

5.6 Relationship Between Probability and Wave Function

We learned in elementary physics that the instantaneous wave intensity of electromagnetic radiation (light) is $\epsilon_0 c E^2$ where E is the electric field. Thus the probability of observing light is proportional to the square of the electric field. In the double-slit light experiment we can be assured that the electric field of the light wave is relatively large at the bright spots on the screen and small in the region of the dark places.

If Young's double-slit experiment is performed with very low intensity levels of light, individual flashes can be seen on the observing screen. We show a simulation of the experiment in Figure 5.18. After only 20 flashes (Figure 5.18a) we cannot make any prediction as to the eventual pattern. But we still know that the **probability** of observing a flash is proportional to the square of the electric field. In elementary physics we calculate this result. If the distance from the central ray along the screen we are observing in an experiment like that depicted in Figure 5.17a is denoted by y, the probability for the photon to be found between y and $y + dy$ is proportional to the intensity of the wave (E^2) times dy. For Young's double-slit experiment, the value of the electric field **E** produced by the two interfering waves is large where the flash is likely to be observed and small where it is not likely to be seen. By counting the number of flashes we relate the energy flux I (called the intensity) of the light to the number flux, N per unit area per unit time, of photons having energy $h\nu$. In the wave description, we have $I = \epsilon_0 c \langle E^2 \rangle$ (where E is the electric field), and in what appears to be the particle description, $I = Nh\nu$. The flux of photons N, or the probability P of observing the photons, is proportional to the average value of the square of the electric field $\langle E^2 \rangle$.

How can we interpret the probability of finding the electron in the wave description? First, let's remember that the localization of a wave can be accomplished by using a wave packet. We used a function $\Psi(x, t)$ to denote the superposition of many waves to describe the wave packet. We call this function $\Psi(x, t)$ the **wave function.** In the case of light, we know that the electric field **E** and magnetic field **B** satisfy a wave equation. In electrodynamics either **E** or **B** serves as the wave function Ψ. For particles (say electrons) a similar behavior occurs. In this case the wave function $\Psi(x, t)$ determines the probability, just as the flux of photons N arriving at the screen and the (electric field) **E** determined the probability in the case of light.

For matter waves having a de Broglie wavelength, it is the wave function Ψ that determines the likelihood (or probability) of finding a particle at a particular position in space at a given time. The value of the wave function Ψ has no physical significance itself, and as we will learn later, it can have a **complex** value. The quantity $|\Psi|^2$ is called the **probability density** and represents the probability of finding the particle in a given unit volume and at a given instant of time.

In general, $\Psi(x, y, z, t)$ is a complex quantity and depends on the spatial coordinates x, y, and z as well as time t. The complex nature will be of no concern to us: we use Ψ times its complex conjugate Ψ^* when finding probabilities. We are only interested here in a single dimension y along the observing screen and for a given time t. In this case $\Psi^*\Psi \, dy = |\Psi|^2 dy$ is the probability of observing an electron in the interval between y and $y + dy$ at a given time, and we call this $P(y)dy$.

$$P(y)dy = |\Psi(y, t)|^2 dy \qquad (5.33)$$

Wave function

The wave function: waves for matter

Probability density

Normalization   Because the electron has to have a probability of unity of being observed *somewhere* along the screen, we integrate the probability density over all space by integrating over y from $-\infty$ to ∞. This process is called *normalization*.

$$\int_{-\infty}^{\infty} P(y)\,dy = \int_{-\infty}^{\infty} |\Psi(y,t)|^2\,dy = 1 \tag{5.34}$$

The probability interpretation of the wave function was first proposed in 1926 by Max Born (Nobel Prize, 1954), one of the founders of the quantum theory. The determination of the wave function $\Psi(x,t)$ will be discussed in much more detail in the next chapter.

The use of wave functions $\Psi(x, y, z, t)$ rather than the classical positions $x(t)$, $y(t)$, $z(t)$ represents a clean break between classical and modern physics. In order to be useful in determining values of physical observables like position, momentum, and energy, a set of rules and procedures has been developed (see Section 6.2).

Example 5.6

Consider a particle of mass m trapped in a one-dimensional box of width ℓ. Calculate the possible energies of the particle. What is the most probable location of the particle in the state with the lowest energy at a given time, say $t = 0$, so that $\Psi(x, 0) = \psi(x)$?

Solution: Let us treat the particle as a sinusoidal wave. The particle cannot physically be outside the confines of the box, so the amplitude of the wave motion must vanish at the walls and outside the box. In the language of the wave function, its probability of being outside is zero, so the wave function must vanish outside. The wave function should be continuous, and the probability distribution can have only one value at each point in the box. Several possible waves are shown in Figure 5.21. An integral number of half wavelengths $\lambda/2$ must fit into the box, so

$$\frac{n\lambda}{2} = \ell \quad \text{or} \quad \lambda_n = \frac{2\ell}{n} \quad n = 1, 2, 3, \ldots \tag{5.35}$$

The possible wavelengths are quantized, and the wave shapes will have $\sin(n\pi x/\ell)$ terms. If we treat the problem nonrelativistically and assume there is no potential energy, the energy E of the particle is

$$E = \text{K.E.} = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}$$

If we insert the values for λ_n, we have

$$E_n = \frac{h^2 n^2}{2m(4\ell^2)} = n^2 \frac{h^2}{8m\ell^2} \quad n = 1, 2, 3, \ldots \tag{5.36}$$

Therefore, the possible energies of the particle are quantized, and the lowest energy $E_1 = h^2/8m\ell^2$. Each of these possible energies is called an **energy level.**

The probability of observing the particle between x and $x + dx$ in each state is $P_n\,dx \propto |\psi_n(x)|^2\,dx$. Notice that $E_0 = 0$ is not a possible state, because $n = 0$ corresponds to $\psi_0 = 0$. The lowest energy level is, therefore E_1 and $P_1 \propto |\psi_1(x)|^2$, shown in Figure 5.21. The most probable location for the particle in the lowest energy state is in the middle of the box.
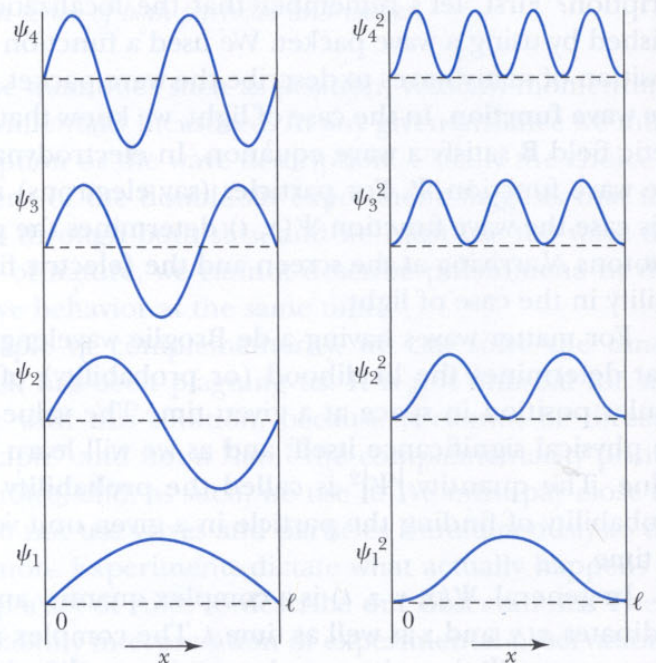

FIGURE 5.21 Possible ways of fitting waves into a one-dimensional box of length ℓ. The left side shows the wave functions for the four lowest energy values. The right side shows the corresponding probability distributions.

The previous example is an important one. It is our first application of quantum theory using waves. Notice how the quantization of energy arises from the need to fit a whole number of half-waves into the box, and how we obtained the corresponding probability densities of each of the states. We reintroduced the concept of energy levels, first discussed in the Bohr model. The procedure followed in the example is the same as finding the allowed modes of standing waves inside the box. We can use all the results that we learned about waves in elementary physics.

5.7   Uncertainty Principle

In Section 5.4, when we discussed the superposition of waves, we learned that in order to localize a wave packet over a small region Δx, we had to use a large range, Δk, of wave numbers. For the case of two waves we found in Equation (5.22) that $\Delta k \, \Delta x = 2\pi$. If we examine a Gaussian wave packet closely, we would find that the product $\Delta k \, \Delta x = 1/2$. The minimum value of the product $\Delta k \, \Delta x$ is obtained when Gaussian wave packets are used.

In Section 5.4 we learned that it is impossible to measure simultaneously, with no uncertainty, the precise values of k and x for the same particle. The wave number k may be rewritten as

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = p\frac{2\pi}{h} = \frac{p}{\hbar} \qquad (5.37)$$

and

$$\Delta k = \frac{\Delta p}{\hbar} \qquad (5.38)$$

so that, in the case of the Gaussian wave packet,

$$\Delta k \, \Delta x = \frac{\Delta p}{\hbar} \Delta x = 1/2$$

or

$$\Delta p \, \Delta x = \hbar/2 \qquad (5.39)$$

for Gaussian wave packets.

The relationship in Equation (5.39) was first enunciated in 1927 by the German physicist Werner Heisenberg, who won the Nobel Prize in 1932. This uncertainty also applies in all three dimensions, so we should put a subscript on Δp to indicate the x direction Δp_x. Heisenberg's **uncertainty principle** can therefore be written

$$\Delta p_x \, \Delta x \geq \hbar/2 \qquad (5.40)$$

Heisenberg uncertainty principle for p_x and x

which establishes limits on the simultaneous knowledge of the values of p_x and x.* The limits on Δp_x and Δx represent the lowest possible limits on the uncertainties in knowing the values of p_x and x, no matter how good an experimental measurement is made. It is possible to have a greater uncertainty in the values of p_x and x, but it is not possible to know them better than allowed by the uncertainty principle. The uncertainty principle does not apply to the products of Δp_z

Werner Heisenberg (1901–1976) was born in Germany where he spent his entire career at various universities including Munich, Leipzig, and Berlin where he was appointed director of the Kaiser Wilhelm Institute in 1942, the highest scientific position in Germany. After World War II Heisenberg spent much of his effort towards supporting research and opportunities for young physicists as well as speaking out against the atom bomb. *AIP Emilio Segrè Visual Archives.*

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*In some representations of the uncertainty principle, the factor $\frac{1}{2}$ is absent. Our form represents the lower limit.

and Δx or to that of Δp_y and Δz. The value of $\Delta p_z \Delta x$ can be zero. Equation (5.40) is true not only for specific waves such as water or sound, but for matter waves as well. It is a consequence of the de Broglie wavelength of matter. If we want to know the position of a particle very accurately, then we must accept a large uncertainty in the momentum of the particle. Similarly, if want to know the precise value of a particle's momentum, it is not possible to specify the particle's location very precisely. The uncertainty principle represents another sharp digression with classical physics, where it is assumed that it is possible to simultaneously specify precisely both the particle's position and momentum. Because of the small value of $\hbar$, the uncertainty principle becomes important only on the atomic level as the following example shows.

Example 5.7

Calculate the momentum uncertainty of (a) a tennis ball constrained to be in a fence enclosure of length 35 m surrounding the court, and (b) an electron within the smallest radius of a hydrogen atom.

Solution: (a) If we insert the uncertainty of the location of the tennis ball, $\Delta x = 35$ m, into Equation (5.39), we have

$$\Delta p \geq \frac{1}{2}\frac{\hbar}{\Delta x} = \frac{1.05 \times 10^{-34}\,\text{J} \cdot \text{s}}{2(35\,\text{m})} = 1.5 \times 10^{-36}\,\text{kg} \cdot \text{m/s}$$

We will have no problem specifying the momentum of the tennis ball!

(b) The diameter of the hydrogen atom in its lowest energy state (smallest radius) is $2a_0$. Let the uncertainty in x be equal to the radius, $\Delta x = a_0$ (even if we let $\Delta x = 2a_0$ the conclusions are valid).

$$\Delta x = a_0 = 0.53 \times 10^{-10}\,\text{m}$$

$$\Delta p \geq \frac{1}{2}\frac{\hbar}{\Delta x} = \frac{1.05 \times 10^{-34}\,\text{J} \cdot \text{s}}{2(0.53 \times 10^{-10}\,\text{m})}$$

$$= 0.99 \times 10^{-24}\,\text{kg} \cdot \text{m/s}$$

It is likely that the momentum of the electron is at least as big as its uncertainty, so we let $p = (\Delta p)_\text{min}$ and calculate the electron's minimum kinetic energy from $p^2/2m$.

$$\text{K.E.} = \frac{p^2}{2m} = \frac{(\Delta p)^2_\text{min}}{2m} = \frac{(0.99 \times 10^{-24}\,\text{kg} \cdot \text{m/s})^2}{(2)(9.11 \times 10^{-31}\,\text{kg})}$$

$$= 5.4 \times 10^{-19}\,\text{J}\left(\frac{1\,\text{eV}}{1.6 \times 10^{-19}\,\text{J}}\right) = 3.4\,\text{eV}$$

Remember that the binding energy of the electron in the hydrogen atom is 13.6 eV, so that on the atomic scale, the uncertainties can be large percentages of typical values themselves. Similarly, from the value of Δp determined above, we calculate

$$\Delta v = \frac{\Delta p}{m} = \frac{0.99 \times 10^{-24}\,\text{kg} \cdot \text{m/s}}{9.1 \times 10^{-31}\,\text{kg}}$$

$$= 1.1 \times 10^6\,\text{m/s} = 0.0036c$$

In Chapter 4 we found $v = 2.2 \times 10^6$ m/s $= 0.0073c$ for this state, so the uncertainty in the velocity is about 50%.

Equation (5.40) is not the only form of the uncertainty principle. We can find another form by using Equation (5.23) from our study of wave motion. When we superimposed two waves to form a wave packet we found $\Delta\omega\,\Delta t = 2\pi$. If we evaluate this same product using Gaussian packets, we will find

$$\Delta\omega\,\Delta t = \frac{1}{2} \tag{5.41}$$

just as we did for the product $\Delta k\,\Delta x$. A relationship like this is easy to understand. If we are to localize a wave packet in a small time Δt (instead of over an infinite

time as for a single wave), we must include the frequencies of many waves in order to have them cancel everywhere but over the time interval Δt. Because $E = h\nu$, we have for each wave,

$$\Delta E = h\,\Delta\nu = h\,\frac{\Delta\omega}{2\pi} = \hbar\,\Delta\omega$$

therefore

$$\Delta\omega = \frac{\Delta E}{\hbar} \qquad \text{and} \qquad \Delta\omega\,\Delta t = \frac{\Delta E}{\hbar}\,\Delta t = \frac{1}{2}$$

We can therefore obtain another form of Heisenberg's uncertainty principle:

$$\Delta E\,\Delta t \geq \frac{\hbar}{2} \qquad\qquad (5.42)$$

Heisenberg uncertainty principle for energy and time

There are other *conjugate variables* similar to p and x in Equation (5.40) that also form uncertainty principle relations. These variables include the angular momentum L and angle θ, for example, as well as the rotational inertia I and angular velocity ω. Similar uncertainty relations can be written for them.

We once again must emphasize that the uncertainties expressed in Equations (5.40) and (5.42) are intrinsic. They are not due to our inability to measure more precisely. No matter how well we can measure, no matter how accurate an instrument we build, and no matter how long we measure, we can never do any better than the uncertainty principle allows. Many people, including Einstein, have tried to think of situations in which it is violated, but they have not succeeded. At the 1927 Solvay conference Bohr and Einstein had several discussions about the uncertainty principle. Every morning at breakfast Einstein would present a new *gedanken* experiment that would challenge the uncertainty principle. In his careful, deliberate manner, Bohr would refute each objection. Eventually Einstein conceded—he could not provide a valid example of contradiction. These discussions continued off and on into the 1930s, because Einstein had difficulty accepting the idea that the quantum theory could give a complete description of physical phenomena. He believed the quantum theory could give a statistical description of a collection of particles but could not describe the motion of a single particle. Einstein presented several paradoxes to support his ideas. Bohr was able to analyze each paradox and present a reasonable answer. Bohr stressed his complementarity principle, which precludes a simultaneous explanation in terms of waves and particles, as well as Heisenberg's uncertainty principle, which surprisingly does allow small violations of the conservation laws of energy and momentum.

Bohr and Einstein discussions

It may seem paradoxical that energy conservation is violated in quantum physics, but no paradox is involved because the energy violation ΔE cannot be detected by any experiment. Suppose that one wishes to observe a deviation from exact energy conservation by an amount ΔE. The uncertainty principle requires that the time during which this violation takes place is on the order of $\Delta t = \hbar/2\Delta E$. To observe a time interval this short, we need a clock ticking at intervals less than Δt, that is, a train of pulses of frequency $\nu = 1/\Delta t$. But the quanta in this wave train have energies $E = h\nu = h/\Delta t = 4\pi\Delta E$, so the wave quanta have plenty of energy to disturb the system by at least the energy ΔE. Any attempt to measure ΔE must disturb the system by at least as much as the uncertainty ΔE.

Let's return to the previous discussion of determining which slit an electron passes through in the double-slit experiment (see Figure 5.20). We again shine light on the electrons passing through the slits and look with a powerful microscope. This time we will use the uncertainty principle and make a more detailed calculation. The light photons bounce off the electron as it passes through one of the slits and scatter into the microscope where we observe them. We must be able to locate the electron's position in y to at least within $\Delta y < d/2$ (where d is the distance between the two slits) in order to know which slit the electron went through. If the position of the electron is uncertain to less than $d/2$, then according to the uncertainty principle, the electron's momentum must be uncertain to at least $\Delta p_y > \hbar/d$. Just by scattering photons off the electrons in order to know which slit the electron went through, we introduce an uncertainty in the electron's momentum. This uncertainty has been caused by the measurement itself.

Consider an electron originally moving in a particular direction; let us choose $\theta = 0$ for convenience. By scattering the photon we now have an uncertainty in the angle θ due to the "kick" given the electron by the photon in the measurement process. The uncertainty in the electron's angle due to a possible momentum change along the y axis is $\Delta\theta = \Delta p_y/p$, but because $p = h/\lambda$, we have

$$\Delta\theta = \frac{\Delta p_y}{p} = \frac{(\Delta p_y)\lambda}{h} = \frac{(\hbar)\lambda}{dh} = \frac{\lambda}{2\pi d}$$

According to Equation (5.32) the first interference maximum will be at $\sin\theta = \lambda/d$ and the first minimum at $\sin\theta = \lambda/2d$. For small angle scattering, $\sin\theta \approx \theta$, and the angle of the first minimum is $\theta_{min} \approx \lambda/2d$. Note that the position of the first minimum is on the same order as our uncertainty in $\Delta\theta$, so the interference pattern is washed out. If we insist on identifying the electrons as particles and knowing which slit the electrons pass through, the wave characteristics of the electron disappear. We cannot simultaneously treat the electron as both a particle and a wave.

This limitation seems to be a fundamental characteristic of the laws of nature. Only the smallness of Planck's constant h keeps us from encountering this limitation in everyday life. Niels Bohr tried to turn this limitation into a philosophical principle. When he was awarded the Danish Order of the Elephant he put on his coat of arms (see Figure 5.22) the Chinese yin-yang symbol, which stands for the two opposing but inseparable elements in nature. The Latin motto on the center of the coat of arms means "Opposites are Complementary."

FIGURE 5.22 Niels Bohr's coat of arms was designed in 1947 when he was awarded the Danish Order of the Elephant. This award was normally given only to royalty and foreign presidents. Bohr chose the Chinese yin-yang symbol because it stands for the two opposing but inseparable elements of nature. The translation of the Latin motto is "Opposites are complementary." It was hung near the king's coat of arms in the church of Frederiksborg Castle at Hillerod. *AIP Niels Bohr Library. Margarethe Bohr Collection.*

Example 5.8

Calculate the minimum kinetic energy of an electron that is localized within a typical nuclear radius of 6×10^{-15} m.

Solution: Let's assume the minimum electron energy is that due to the uncertainty principle with an uncertainty Δx equal to the radius ($\Delta x = \pm r$).

$$\Delta x \approx r = 6 \times 10^{-15} \text{ m}$$

$$\Delta p \geq \frac{\hbar}{2\Delta x} = \frac{6.58 \times 10^{-16} \text{ eV} \cdot \text{s}}{1.2 \times 10^{-14} \text{ m}}$$

$$\geq 5.48 \times 10^{-2} \text{ eV} \cdot \text{s/m} \frac{3 \times 10^8 \text{ m/s}}{c}$$

$$\geq 1.64 \times 10^7 \text{ eV}/c$$

Let's now assume that the momentum p is at least as large as the uncertainty in p.

$$p \approx \Delta p \geq 1.64 \times 10^7 \text{ eV}/c$$

Because we don't yet know the electron's energy, let's be careful and calculate it relativistically.

$$E^2 = (pc)^2 + E_0^2$$

$$= \left[\left(1.64 \times 10^7 \frac{\text{eV}}{c}\right)c\right]^2 + (0.511 \text{ MeV})^2$$

$$= (16.4 \text{ MeV})^2 + (0.511 \text{ MeV})^2$$

$$E = 16.4 \text{ MeV}$$

$$\text{K.E.} = E - E_0 = 16.4 \text{ MeV} - 0.51 \text{ MeV}$$

$$= 15.9 \text{ MeV}$$

Note that because K.E. $> E_0$, a relativistic calculation was actually needed. This value of K.E. is larger than that observed for electrons emitted from nuclei in beta decay. We must conclude that electrons cannot be confined within the nucleus. Electrons emitted from the nucleus (during beta decay) must actually be created when they are emitted.

Example 5.9

An atom in an excited state normally remains in that state for a very short time ($\sim 10^{-8}$ s) before emitting a photon and returning to a lower energy state. The "lifetime" of the excited state can be regarded as an uncertainty in the time Δt associated with a measurement of the energy of the state. This, in turn, implies an "energy width," namely, the corresponding energy uncertainty ΔE. Calculate the characteristic "energy width" of such a state.

Solution: Because $\Delta E \, \Delta t \geq \hbar/2$

$$\Delta E \geq \frac{\hbar}{2\Delta t} = \frac{6.58 \times 10^{-16} \text{ eV} \cdot \text{s}}{(2)(10^{-8} \text{ s})} = 3.3 \times 10^{-8} \text{ eV}$$

This is a very small energy, but many excited energy states have such energy widths. For stable ground states, $\tau = \infty$, and $\Delta E = 0$. For excited states in the nucleus, the lifetimes can be as short as 10^{-20} s (or shorter) with energy widths of 100 keV (or more).

Summary

Max von Laue suggested the scattering of x rays from matter, thereby firmly establishing the wave nature of x rays and the lattice structure of crystals. W. H. Bragg and W. L. Bragg exploited the wave behavior of x rays by utilizing x-ray scattering to determine the spacing d between crystal planes according to Bragg's law

$$n\lambda = 2d \sin \theta \tag{5.1}$$

In an important conceptual leap, de Broglie suggested that particles might also exhibit wave properties, with a wavelength λ determined by their momentum

$$\lambda = \frac{h}{p} \qquad \text{de Broglie wavelength} \tag{5.2}$$

Davisson and Germer, and G. P. Thomson independently, demonstrated the wave characteristics of particles by diffracting low-energy electrons from crystals.

Particles may be described using waves by representing them as wave packets, the superposition of many waves of different amplitudes and frequencies. The group velocity $u_{gr} = d\omega/dk$ represents the speed of the particle described by the wave packet.

Niels Bohr proposed a principle of complementarity, stating that it is not possible to describe physical behavior simultaneously in terms of both particles and waves. We must use either one form of description or the other. This principle avoids the conceptual wave–particle duality problem by precluding a simultaneous description of experiments by both wave and particle behavior.

We describe particles exhibiting wave behavior by using wave functions Ψ, which in general may be complex-valued functions of space and time. The probability of observing a particle between x and $x + dx$ at time t is $|\Psi(x, t)|^2 dx$.

Werner Heisenberg pointed out that it is not possible to know simultaneously both the exact momentum and position of a particle or to know its precise energy at a precise time. These relationships

$$\Delta p_x \, \Delta x \geq \hbar/2 \tag{5.40}$$

$$\Delta E \, \Delta t \geq \hbar/2 \tag{5.42}$$

are called *Heisenberg's uncertainty principle* and are consistent with Bohr's complementarity principle. No experiment, regardless of how clever, can measure p, x, E, and t better than the uncertainties expressed in Equations (5.40) and (5.42).

Questions

1. In 1900 did it seem clear that x rays were electromagnetic radiation? Give reasons why you think so. Was it important to perform further experiments to verify the characteristics of x rays?

2. In the early 1900s it was found that x rays were more difficult to refract or diffract than visible light. Why did this lead researchers to suppose that the wavelengths of x rays were shorter rather than longer than those of light?

3. What determines whether a given photon is an x ray? Could an x ray have a wavelength longer than ultraviolet light?

4. For a single crystal, transmission x-ray scattering will produce dots. However, if there are randomly oriented crystals, as in powder, concentric rings appear. Explain the difference qualitatively.

5. How many particles can you think of that might be shown experimentally to exhibit wavelike properties? List at least three and discuss possible experiments.

6. Why are neutrons more widely used than protons for studying crystal structure? What about using a hydrogen atom?

7. Why is it important to use "cold" neutrons for studying crystal structure? How could one obtain "cold" neutrons?

8. Are the following phenomena wave or particle behaviors? Give your reasoning (a) television picture, (b) rainbows on a rainy day, (c) football sailing through goal posts, (d) telescope observing the moon, (e) police radar.

9. The experiment by Jönsson that showed the wavelike properties of electrons passing through a double slit is considered a pedagogically interesting experiment but not a landmark experiment. Why do you suppose this is true?

10. Can you think of an experiment other than those mentioned in this chapter that might show the wavelike properties of particles? Discuss it.

11. Why doesn't the uncertainty principle restriction apply between the variables p_z and x?

12. How does the uncertainty principle apply to a known stable atomic system that apparently has an infinite lifetime? How well can we know the energy of such a system?

13. According to the uncertainty principle, can a particle having a kinetic energy of exactly zero be confined somewhere in a box of length ℓ? Explain.

14. What is similar about the conjugate variable pairs (p, x), (E, t), (L, θ), and (I, ω)?

15. What are the dimensions of the wave function $\Psi(x, t)$ that describes matter waves? Give your reasoning.

16. Soon after their discovery, Davisson and Germer were using their experimental technique to point out new crystal structures of nickel. Do you think they were justified? Explain how you think their results allowed them to make such statements.

Problems

5.1 X-Ray Scattering

1. X rays scattered from a crystal have a first-order diffraction peak at $\theta = 15°$. At what angle will the second- and third-order peaks appear?

2. X rays of wavelength 0.16 nm are scattered from NaCl. What is the angular separation between first- and second-order diffraction peaks? Assume scattering planes that are parallel to the surface.

3. Potassium chloride is a crystal with lattice spacing of 0.314 nm. The first peak for Bragg diffraction occurs at 14°. What energy x rays were diffracted? What other order peaks can be observed ($\theta \le 90°$)?

4. A cubic crystal with interatomic spacing of 0.24 nm is used to select γ rays of energy 100 keV from a radioactive source containing a continuum of energies. If the incident beam is normal to the crystal, at what angle do the 100-keV γ rays appear?

5.2 De Broglie Waves

5. Calculate the de Broglie wavelength of a 3.0 kg rock thrown with a speed of 6 m/s into a pond. Is this wavelength similar to that of the water waves produced? Explain.

6. Calculate the de Broglie wavelength of a nitrogen molecule in the atmosphere on a hot summer day (35°C). Compare this with the diameter (less than 1 nm) of the molecule.

7. Work out Example 5.2b strictly using SI units of m, J, kg, and so on, and compare with the method of the example using eV units.

8. Assume that the total energy E of an electron greatly exceeds its rest energy. If a photon has a wavelength equal to the de Broglie wavelength of the electron, what is the photon's energy? What if $E = 2E_0$ for the electron?

9. Determine the de Broglie wavelength of a particle of mass m and kinetic energy K. Do this for both (a) a relativistic and (b) a nonrelativistic particle.

10. The Stanford Linear Accelerator can accelerate electrons to an energy of 50 GeV. What is the de Broglie wavelength of these electrons? What fraction of a proton's diameter ($d \sim 2 \times 10^{-15}$ m) can such a particle probe?

11. Find the kinetic energy of (a) photons, (b) electrons, (c) neutrons, and (d) α particles that have a de Broglie wavelength of 0.15 nm.

12. Find the de Broglie wavelength of neutrons in equilibrium at the temperatures (a) 10 K and (b) 0.1 K.

13. An electron initially at rest is accelerated across a potential difference of 3 kV. What are its wavelength, momentum, kinetic energy, and total energy?

14. What is the wavelength of an electron with kinetic energy (a) 40 eV, (b) 400 eV, (c) 4 keV, (d) 40 keV, (e) 0.4 MeV, and (f) 4 MeV? Which of these energies are most suited for study of the NaCl crystal structure?

15. Calculate the de Broglie wavelength of (a) an oxygen (O_2) molecule darting around the room at 480 m/s, (b) a bacterium of mass 1.5×10^{-15} kg moving at a speed of 10^{-6} m/s.

16. What is the de Broglie wavelength of the 1 TeV protons accelerated in the Fermi National Laboratory Tevatron accelerator?

5.3 Electron Scattering

17. In an electron-scattering experiment an intense reflected beam is found at $\phi = 32°$ for a crystal with an interatomic distance of 0.23 nm. What is the lattice spacing of the planes responsible for the scattering? Assuming first-order diffraction, what are the wavelength, momentum, kinetic energy, and total energy of the incident electrons?

18. Davisson and Germer performed their experiment with a nickel target for several energies. At what angles would they find diffraction maxima for 48-eV and 64-eV electrons?

19. A beam of 2-keV electrons incident on a crystal is refracted and observed (by transmission) on a screen 35 cm away. The radii of three concentric rings on the screen, all corresponding to first-order diffraction, are 2.1 cm, 2.3 cm, and 3.2 cm. What is the lattice-plane spacing corresponding to each of the three rings?

20. A beam of thermal neutrons (K.E. = 0.025 eV) scatters from a crystal with interatomic spacing 0.45 nm. What is the angle of the first-order Bragg peak?

5.4 Wave Motion

21. A wave, propagating along the x direction according to Equation (5.11), has a maximum displacement of 3 cm at $x = 0$ and $t = 0$. The wavespeed is 4 cm/s, and the wavelength is 7 cm. (a) What is the frequency? (b) What is the wave's amplitude at $x = 10$ cm and $t = 13$ s?

22. A wave of wavelength 4 cm has a wavespeed of 4 cm/s. What is its (a) frequency (b) period (c) wave number and (d) angular frequency?

23. Two waves are traveling simultaneously down a long slinky. They can be represented by $\Psi_1(x, t) = 0.003 \sin(6.0x - 300t)$ and $\Psi_2(x, t) = 0.003 \sin(7.0x - 250t)$. Distances are measured in meters and time in seconds. (a) Write the expression for the resulting wave. (b) What are the phase and group velocities? (c) What is Δx between two adjacent zeros of Ψ? (d) What is $\Delta k \, \Delta x$?

24. A wave packet describes a particle having momentum $p = mv$. Show that the group velocity is βc and the phase velocity is c/β (where $\beta = v/c$). How can the phase velocity physically be greater than c?

25. For waves in shallow water the phase velocity is about equal to the group velocity. What is the dependence of the phase velocity on the wavelength?

26. Find the group and phase velocities of 8-MeV protons and 8-MeV electrons (see Problem 24).

27. Use Equation (5.25) with $\tilde{A}(k) = A_0$ for the range of $k = k_0 - \Delta k/2$ to $k_0 + \Delta k/2$ and $\tilde{A}(k) = 0$ elsewhere to determine $\Psi(x, 0)$, that is, at $t = 0$. Sketch the envelope term, the oscillating term, and $|\Psi(x, 0)|^2$. What is approximately the width Δx over the full-width–half-maximum part of $|\Psi(x, 0)|^2$? What is the value of $\Delta k \, \Delta x$?

28. Show using Equation (5.29) that u_{gr} correctly represents the velocity of the particle both relativistically and classically.

5.5 Waves or Particles?

29. Light of intensity $\mathcal{I}_0$ passes through two sets of apparatus. One contains one slit and the other two slits. The slits have the same width. What is the ratio of the outgoing intensity amplitude for the central peak for the two-slit case compared to the single slit?

30. Design a double-slit electron-scattering experiment using 1-keV electrons that will provide the first maximum at an angle of 1°. What will be the slit separation d?

31. You want to design an experiment similar to the one done by Jönsson that does not require magnification of the interference pattern in order to be seen. Let the two slits be separated by 2000 nm. Assume that you can discriminate visually between maxima that are as little as 0.3 mm apart. You have at your disposal a lab that allows the screen to be placed 80 cm away from the slits. What energy electrons will you require? Do you think such low-energy electrons will represent a problem? Explain.

5.6 Relationship Between Probability and Wave Function

32. The wave function of a particle in a one-dimensional box of length L is $\Psi(x) = A \sin(\pi x/L)$. If we know the particle must be somewhere in the box, what must be the value of A?

33. A particle in a one-dimensional box of length L has a kinetic energy much greater than its rest energy. What is the ratio of the energy levels E_n: E_2/E_1, E_3/E_1, E_4/E_1? How do you explain this result?

34. Write down the normalized wave functions for the first three energy levels in Example 5.6. Assume there are equal probabilities of being in each state.

5.7 Uncertainty Principle

35. A neutron is confined in a deuterium nucleus (deuteron) of diameter $\approx 2 \times 10^{-15}$ m. Use the energy-level calculation of a one-dimensional box to calculate the neutron's minimum kinetic energy. What is the neutron's minimum kinetic energy according to the uncertainty principle?

36. What is the ratio uncertainty of the velocities ($\Delta v/v$) of (a) an electron and (b) a proton confined to a one-dimensional box of length 2 nm?

37. Show that the uncertainty principle can be expressed in the form $\Delta L \, \Delta\theta \geq \hbar/2$, where θ is the angle and L the angular momentum. For what uncertainty in L will the angular position of a particle be completely undetermined?

38. Some physics theories indicate that the lifetime of the proton is about 10^{36} years. What would such a prediction say about the energy of the proton?

39. What is the bandwidth $\Delta\omega$ of an amplifier for radar if it amplifies a pulse of width 2 μs?

40. Find the minimum uncertainty in the speed of a bacterium having mass 3×10^{-15} kg if we know the position of the bacterium to within 1 micron, that is, to about its own size.

41. An atom in an excited state of 4.7 eV emits a photon and ends up in the ground state. The lifetime of the excited state is 10^{-13} s. (a) What is the energy uncertainty of the emitted photon? (b) What is the spectral line width (in wavelength) of the photon?

42. An electron microscope is designed to resolve objects as small as 0.14 nm. What energy electrons must be used in this instrument?

43. Rayleigh's criterion is used to determine when two objects are barely resolved by a lens of diameter d. The angular separation must be greater than θ_R where

$$\theta_R = 1.22 \frac{\lambda}{d}$$

In order to resolve two objects 4000 nm apart at a distance of 20 cm with a lens of diameter 5 cm, what energy (a) photons or (b) electrons should be used? Is this consistent with the uncertainty principle?

44. Calculate the de Broglie wavelength of a 5.5-MeV α particle emitted from an ^{241}Am nucleus. Could this particle exist inside the ^{241}Am nucleus (diameter $\approx 1.6 \times 10^{-14}$ m)?

45. Show that the minimum energy of a simple harmonic oscillator is $\hbar\omega/2$. What is the minimum energy in joules for a mass of 2 g oscillating on a spring with a spring constant 8 N/m?

General Problems

46. Consider a wave packet having the product of $\Delta p \, \Delta x = \hbar$ at a time $t = 0$. What will be the width of such a wave packet after the time $m(\Delta x)^2/\hbar$?

47. Analyze the Gaussian wave packet carefully and show that $\Delta k \, \Delta x = 1/2$. You must justify the assumptions you make concerning uncertainties in k and x. Take the Gaussian form given in Equation (5.26). (*Hint*: the linear "spread" of the wave packet Δx is given by one standard deviation, at which point the probability amplitude ($|\Psi|^2$) has fallen to one half its peak value.)

48. Most of the particles known to physicists are unstable. For example the lifetime of the neutral pion, π^0, is about 10^{-16} s. Its mass is 135 MeV/c^2. What is the energy width of the π^0 in its ground state?

49. The range of the nuclear strong force is believed to be about 1.2×10^{-15} m. The particle that "mediates" the strong force (similar to the photon mediating the electromagnetic force) is the pion. Assume that the pion moves at the speed of light in the nucleus, and calculate the time Δt it takes to travel between nucleons. Assume that the distance between nucleons is also about 1.2×10^{-15} m. Use this time Δt to calculate the energy ΔE for which energy conservation is violated during the time Δt. This ΔE has been used to estimate the mass of the pion. What value do you determine for the mass? Compare this value with the measured value of 135 MeV/c^2 for the neutral pion.

50. The planes of atoms in a cubic crystal lie parallel to the surface, 0.8 nm apart. X rays having wavelength 0.5 nm are directed at an angle θ to the surface. (a) For what values of θ will there be a strong reflection? (b) What energy electrons could give the same result?

51. Aliens visiting Earth are fascinated by baseball. They are so advanced that they have learned how to vary $\hbar$ to make sure that a pitcher cannot throw a strike with any confidence. Assume the width of the strike zone is 0.38 m, the speed of the baseball is 35 m/s, the mass of the baseball is 145 g, and the ball travels a distance of 18 m. What value of $\hbar$ is required? (*Hint*: there are two uncertainties here: the width of the strike zone and the transverse momentum of the pitched ball.)