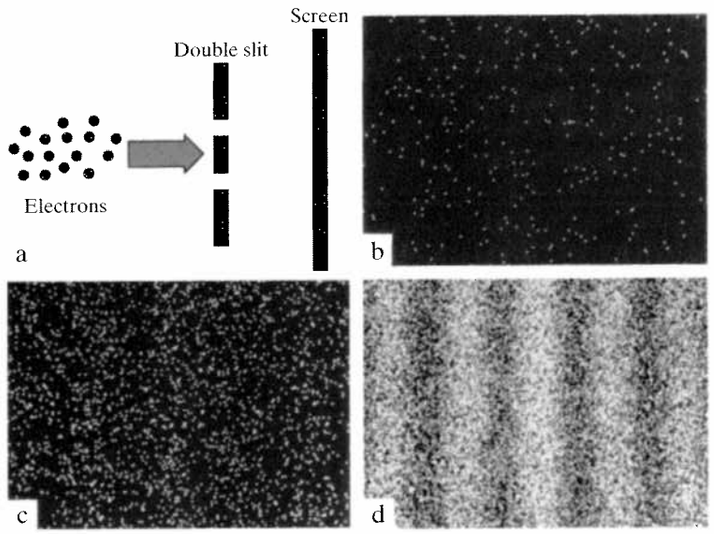
Chapter

2

CLASSICAL PARTICLES, CLASSICAL WAVES, AND QUANTUM PARTICLES



Experimental diffraction pattern of the classic double-slit experiment, applied to electrons. (Based on Tonomura, A., et al., "Demonstration of Single-Electron Build-Up of an Interference Pattern," *Am. J. Phys.* 57 (1989): 117. Courtesy of the American Institute of Physics. © Hitachi Ltd. Advanced Research Laboratory.)

This chapter provides a brief review of a few concepts from classical (Newtonian) physics, and presents some aspects of quantum phenomena that are important in understanding nanoelectronics. A few experiments are discussed that show the inadequacy of classical physics in explaining some aspects of light and matter. However, these experiments are not merely historical. They illustrate some basic properties of what will be called *quantum particles* (a designation that covers both light and electrons), and, in fact, some of these experiments point the way towards novel devices and new technologies.

2.1 COMPARISON OF CLASSICAL AND QUANTUM SYSTEMS

A classical particle is what we think of as an ordinary particle or object, such as a billiard ball, a car, or a bullet. Of course, a classical particle with mass m occupies a definite position in space, $\mathbf{r}(t)$ at a time t (this position indicates, perhaps, the center of mass of the object). For example, in rectangular coordinates, the position of a particle can be given by

$$\mathbf{r}(t) = \mathbf{a}_x x(t) + \mathbf{a}_y y(t) + \mathbf{a}_z z(t), \tag{2.1}$$

where $\mathbf{a}_x$, $\mathbf{a}_y$, and $\mathbf{a}_z$ are unit vectors along the x, y, and z coordinates, respectively. If the particle is moving along a trajectory T, it has a definite velocity, $\mathbf{v} = d\mathbf{r}(t)/dt$, as shown in Fig. 2.1, and the particle has a definite momentum, $\mathbf{p} = m\mathbf{v}$, and definite acceleration, $\mathbf{a} = d^2\mathbf{r}(t)/d^2t$. Note that in this text, vectors are denoted by boldface symbols.

Classical particles obey Newtonian mechanics,

$$\mathbf{F} = m\frac{d^2\mathbf{r}}{dt^2}, \tag{2.2}$$

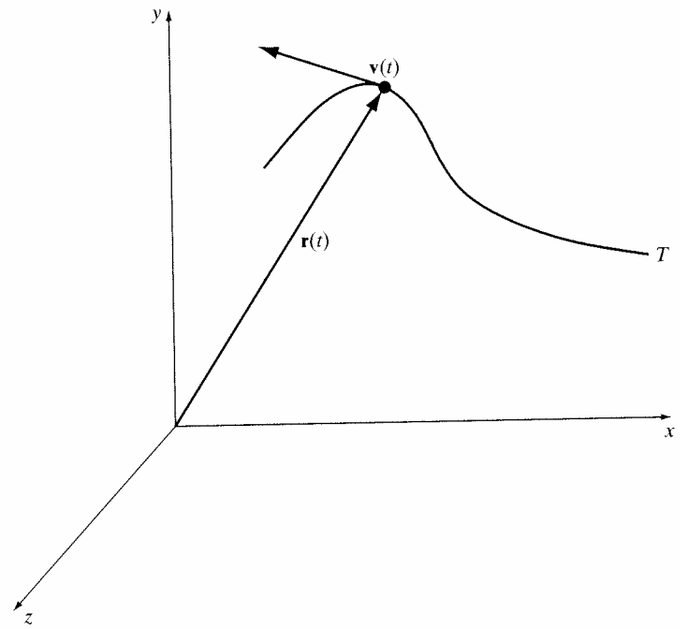


Figure 2.1 A classical particle trajectory T; the particle is located by position $\mathbf{r}(t)$ and has velocity $\mathbf{v}(t)$.

where **F** is an applied force, either mechanical or electrical. In classical physics, physical quantities such as position and momentum can, in principle, be measured with absolute certainty. Using (2.2), we can, in principle, determine with certainty the particle's trajectory for all future times from a set of initial conditions. For systems containing hundreds or perhaps billions of particles, all interacting with each other via collisions and mutual attractions and repulsions, one can still determine, in principle, how each particle will behave in space and time.

The (over)use of the words "in principle" and "definite" in the preceding paragraphs demands some explanation. The point is that the described calculations based on Newton's laws can be, in principle, performed, although it may be extremely difficult to do so. As an example, consider the seemingly simple problem of a ball being thrown through the air. This is actually a very difficult process to model because of the complicated (and often unknown) form of the force term in (2.2). Air molecules, pollution, wind, rain, etc., act as forces on the ball, making its trajectory virtually impossible to determine without simplifying assumptions. For example, perhaps we can assume that friction with air molecules can be ignored, and that there is no wind or rain. In this case, there is, perhaps, only the force of gravity. With such simplifying assumptions, the resulting equation can easily be solved, although whether or not such a simplified problem models physical reality is an important consideration.

In actuality, many of the things that were just mentioned as forces can be thought of as other particles (e.g., air molecules and rain drops), with the result that the force term in Newton's law may be simplified at the expense of keeping track of the mutual interactions among, perhaps, millions or billions of particles. However, given enough computational power, the problem can be solved. On the other hand, for systems having an extremely large number of particles (say, a gas or a liquid), one can obtain information about measurable quantities such as pressure and energy using statistical techniques, which approximate the particle physics in a tractable way.

In the first paragraph of this section, the word "definite" was also used quite a bit, perhaps so much so as to be distracting. However, that was, in fact, the point. Classical physics is characterized by being able to exactly state where a particle will be, and how fast it will be going, at a certain instant of time.[†] However, the actual computation may be difficult or practically impossible to perform.

Quantum mechanics, on the other hand, indicates a quite different situation. Stated briefly, quantum mechanics states that one can only know the probability of a particle being at a certain position at a certain time. It also indicates that it is impossible to measure precisely both the position and momentum of a particle—not that it is really hard to do, but that it is theoretically impossible! For example, the more accurately position is measured, the less will be known about velocity. Perhaps what is most disturbing is that quantum mechanics indicates that there is no such thing as a particle, in the classical sense. All such objects (billiard balls, bullets, electrons, etc.) exhibit properties usually associated with waves, and properties usually associated with particles, the so-called *particle–wave duality*.

[†]With this definition, we are somewhat glossing over things like chaotic effects, where often the system is too sensitive on initial conditions to render a definite answer in practical circumstances.

In a mathematical sense, this leads to particles in quantum theory having a phase component, which will be described in the next chapter.

There are many other disturbing (to our intuition) aspects of quantum theory, some of which will be discussed in this book. One aspect of quantum theory that should be appreciated at the utset is that quantum theory is truly a probabilistic theory. This is in contradistinction to much of what one usually considers to be probabilistic systems. Take, for example, the act of rolling a die. If we know the initial position and momentum of the die, properties of the air through which the die travels, and properties of the surface on which the die lands, etc., we could determine, in principle, what side of the die will face up when the die comes to a stop. However, statistical techniques (e.g., the probability of any given side facing up on a six-sided fair die is 1/6) are used to model this extremely complicated, yet deterministic, problem.[†]

In contrast, quantum mechanics yields quantities that are truly probabilistic. This may indicate a truly probabilistic reality, or perhaps it is merely a probabilistic model of a deterministic reality. As we approach a century of quantum theory, there is still debate on this point; however, it can be safely stated that quantum mechanics is one of the most successful theories ever developed in physics. Philosophy aside, quantum mechanics is currently the only way to model very small (atomic and nanoscopic) objects and devices.

2.2 ORIGINS OF QUANTUM MECHANICS

There are many fine accounts of the development of quantum theory, thanks in part to the fact that quantum theory was developed relatively recently, in the early 1900s. The short and simplified story is that quantum mechanics arose out of experiments performed in the late 1800s and early 1900s that could not be explained by classical physics. In this chapter, the development of quantum theory is not described in any detail, although a few of the basic experiments are described that led to the development of quantum theory, and that, in particular, show the dual wave–particle nature of light, electrons, and, in fact, of all objects. Understanding the wave properties of electrons, that is, that electrons are not small, hard, charged balls but rather (perhaps loosely) localized bundles of energy, is absolutely essential to understanding the fundamental principles of nanoelectronics.

Key to the development of quantum theory were experiments in the 1890s that showed that the specific heat of metals, and thermal blackbody radiation, could not be explained by classical thermodynamics. In addition, in 1887, Heinrich Hertz observed what came to be known as the *photoelectric effect*. Stated briefly, if light is incident on a metal, some energy carried by the light can be transferred to electrons at the metal's surface, and they then may have enough energy to escape from the metal. Classical electromagnetic theory (itself a relatively new discipline at the time) considers light as an electromagnetic wave, and the energy carried by the wave only depends on its amplitude (or intensity), not on its frequency. So if light is indeed a wave phenomenon, experiments

[†]Of course, actually the die is, itself, a quantum object, but we can ignore this fact due to its relatively large mass.

should show that the energy of photo-emitted electrons increases as the intensity of the light increases. However, experiments performed by Philipp Lenard in 1902 showed that this was not the case. Although more electrons were emitted from the metal as the light intensity was increased, the kinetic energy of each emitted electron did not change with intensity. However, when the frequency of the light was increased (i.e., the wavelength was decreased), more energetic electrons were emitted from the metal's surface. Thus, the energy of the emitted electrons was proportional to the incident light's frequency, not to its amplitude.

Furthermore, if light is a wave, then some time should elapse between when the metal is first illuminated and when electrons are first emitted, since a wave continuously transfers energy to the electrons and it should take some time for enough energy to build up to allow the electrons to escape. This was also not found to be the case—sometimes electrons were emitted as soon as the metal was illuminated by the light. There was clearly some problem in how this interaction was being modeled by classical physics.

2.3 LIGHT AS A WAVE, LIGHT AS A PARTICLE

As mentioned above, at the time of the experiments involving the photoelectric effect, light was generally considered to be a wave phenomenon. It is worthwhile to take a brief detour to discuss how this state of knowledge developed.

2.3.1 Light as a Particle, or Perhaps a Wave—The Early Years

Investigations into the nature of light have a long history, not surprisingly. One of the earliest accounts is by Euclid around 300 B.C., who, in his work *Optica*, noted that light travels in straight lines, and described the law of reflection. Jumping far ahead, we find that the 1600s were a particularly important period in the history of light, with such figures as René Descartes, Pierre de Fermat, and Robert Hooke contributing to the field. In 1678, Christiaan Huygens developed a fairly comprehensive wave theory of light, which was very successful in explaining many of the characteristics of light known at the time. Then, in 1704, Isaac Newton, in his work *Opticks*, put forward his view that light is corpuscular in nature, based primarily on the appearance of light traveling in straight lines (since waves can bend around objects to some degree), although he also discussed a wave theory of light. Both the corpuscular and wave theories of light could seemingly be used to explain much of the light phenomena known at the time, such as reflection and refraction.

2.3.2 A Little Later—Light as a Wave

In 1801, Thomas Young performed his famous double-slit experiment, showing evidence for the wave theory of light by demonstrating interference. He was motivated by his earlier work with sound waves, which are known to interfere with each other. In order to grasp the importance of Young's experiment, the concept of interference must first be understood.

Interference. Interference obviously describes the interaction among two or more entities. Let's first consider the familiar example of unit amplitude plane waves, represented as

$$\psi(z) = e^{ikz}, \tag{2.3}$$

where k is a constant called the *wavenumber* (to be discussed later), $i = \sqrt{-1}$ is the imaginary unit, and z is the position coordinate, in this case, the distance that the wave has traveled. We use the symbol ψ to represent the wave, since this notation is generally used in quantum mechanics.

Assume that two plane waves are present, as shown in Fig. 2.2, with the wave represented by ψ_1 emanating from the origin and the wave ψ_2 from the position $z = -L$. Wave ψ_1 travels a distance d to reach the measurement plane, whereas wave ψ_2 must travel a distance $L + d$ to reach the same point. At the position of the measurement plane, the total field ψ_T (i.e., the sum of the waves) is

$$\begin{aligned}\psi_T = \psi_1 + \psi_2 &= e^{ikd} + e^{ik(L+d)} \\ &= e^{ikd}\left(1 + e^{ikL}\right).\end{aligned} \tag{2.4}$$

If

$$kL = 0, 2\pi, 4\pi, \ldots, \qquad |\psi_T| = 2, \tag{2.5}$$

and if

$$kL = \pi, 3\pi, 5\pi \ldots, \qquad |\psi_T| = 0. \tag{2.6}$$

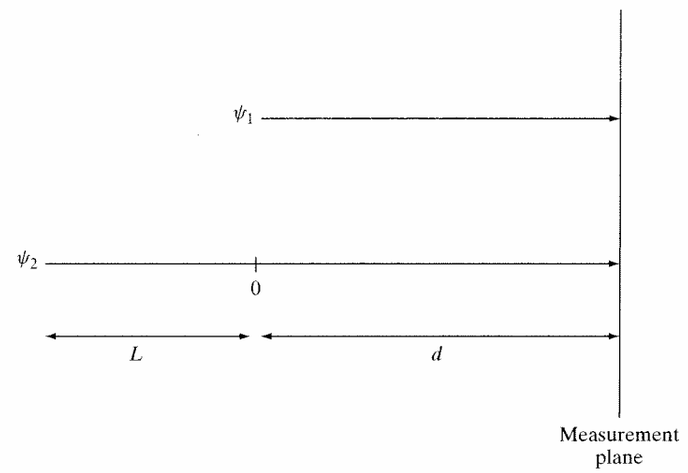


Figure 2.2 Plane waves traveling different distances, resulting in constructive/destructive interference.

That is, at points where the two waves are completely out of phase with each other (i.e., their phase difference is an odd multiple of 180°), they cancel each other out, which is called *destructive interference*. At points where the phase difference is an even multiple of 180°, they add together, doubling their value, which is called *constructive interference*. Therefore, depending of the distance L, the two waves may experience destructive or constructive interference at the measurement plane, or something in between. One can also obtain constructive and destructive interference by combining forward and backward traveling waves,

$$\psi_T = e^{ikz} + e^{-ikz} = 2\cos(kz), \tag{2.7}$$

or

$$\psi_T = e^{ikz} - e^{-ikz} = 2i\sin(kz), \tag{2.8}$$

using Euler's identity ($e^{\pm i\alpha} = \cos\alpha \pm i\sin\alpha$), such as occurs for vibrational waves on guitar strings.

Moreover, more than two plane waves, or other wave types, can be combined to yield constructive and destructive interference. A common example of light interference is a soap film.

The wall thickness of a typical soap film is several microns. The difference in the distance that light must travel in reflecting from the film's top surface, and from the film's bottom surface, is analogous to the difference in distance L depiction in Fig. 2.2. Thus, light reflected from the top surface of the soap film can interfere both constructively and destructively with light reflected from the bottom surface of the film. Since white light is composed of many wavelengths, at any point on the film where wavelengths (i.e., colors) interfere constructively, those colors will be intensified. At points on the film where wavelengths combine destructively, those colors will be suppressed. Thickness variations and other irregularities of the film's surface contribute to the formation of interesting patterns.

Young's Experiment—What to Expect from Waves. Now, getting back to Young's experiment, imagine that two narrow slits are cut into a thin sheet of opaque material, such as metal. A single-frequency (monochromatic) plane wave of light ψ is normally incident on the double slits, as shown in Fig. 2.3.

According to Huygens's principle, each slit reradiates a spherical wave centered on the slit, having the same frequency as the original wave. The waves emanating from slit 1 (the top slit) and slit 2 (the bottom slit) will be denoted by ψ_1 and ψ_2, respectively,

$$\psi_j = A_j \frac{e^{ikr_j}}{r_j}, \tag{2.9}$$

where A_j, $j = 1, 2$, is the amplitude of the wave (if the two slits are equal in size, $A_1 = A_2 = A$), and where r_j is the distance from the center of the jth slit to a given point on the

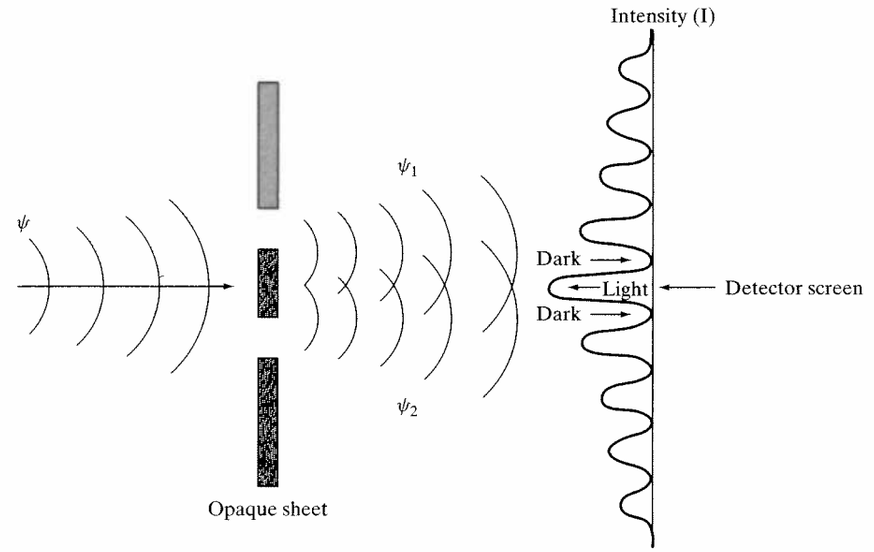


Figure 2.3 Young's double-slit experiment. Incident wave ψ causes spherical waves ψ_1 and ψ_2 to travel toward the detector screen. The resulting intensity pattern I shows interference effects, characteristic of wave behavior.

detector screen. The spherical waves ψ_1 and ψ_2 combine together, such that at any point on the detector screen,

$$\psi_T = A\left(\frac{e^{ikr_1}}{r_1} + \frac{e^{ikr_2}}{r_2}\right), \tag{2.10}$$

forming an interference pattern on the screen (detector) placed behind the slits. That is, at some points on the detector screen the waves ψ_1 and ψ_2 tend to cancel each other out, resulting in destructive interference and a dark patch on the screen. On the other hand, if the waves combine together constructively, a bright patch occurs on the screen.

The location on the screen that lies exactly opposite to the center point of the two slits will be associated with a bright spot, since the two waves travel the same distance from each slit to reach this point. Therefore, they are in phase at this point. Whether or not a particular location on the screen is bright or dark depends on the path difference that the two waves travel to reach the screen. The locations of bright and dark spots can be calculated if the wavelength of the light is known, although the details will be omitted here. However, the resulting bright and dark bands on the screen depicted in Fig. 2.3 show the interference effect, and seemed to be, at the time, conclusive evidence that light is a wave phenomenon. In 1816, Augustin Jean Fresnel presented a mathematically rigorous treatment of the diffraction and interference of light, showing that these phenomena can be explained mathematically by a wave theory of light. Several years later, in 1849, the (seemingly)

final death blow to the particle theory of light was dealt by experiments showing that light propagates more slowly through water than though air—the particle theory of light at the time could only account for the law of refraction if light propagated faster through a dense medium, such as water, than through a more rarefied medium, such as air. So, by the mid 1800s, it seemed clear that light was a wave.

Around the same time, pioneers in electromagnetic theory, such as André Marie Ampère, Michael Faraday, and Carl Gauss, were developing the fields of electricity and magnetism, culminating in the development of Maxwell's equations by James Clerk Maxwell in the 1860s. It was found that the speed of an electromagnetic wave is the same as the speed of light, explaining light as an electromagnetic wave. From Maxwell's equations, one can show that the wave nature of light is revealed when the characteristic dimensions of a system are on the order of, or smaller, than the wavelength of light. When the opposite is true, that is, when the system's dimensions are large compared to wavelength, light appears to exhibit ray-like qualities. This explains why the particle versus wave debate went on for such a long time in the development of optics—in some situations, light does act like a particle, or at least a ray, traveling in straight-line trajectories, and in other situations, light does behave as a wave, exhibiting diffraction.

Therefore, by the late 1800s, the matter seemed settled. A comprehensive mathematical theory had been developed (electromagnetics) showing that light was a wave, and explaining light's ray-like behavior at high frequencies. Electromagnetic theory then continued to be developed, and in the 1890s and early 1900s, Heinrich Hertz, Guglielmo Marconi, and others developed communications aspects of electromagnetic waves, leading to today's radio, telephone, television, and radar, and to a host of other applications. However, at about the same time when it was thought that the debate about the nature of light (and all electromagnetic energy) was finally settled, a scientific revolution was about to take place.

2.3.3 Finally, Light as a Quantum Particle

Before describing some problems with the wave theory of light, we need to consider the double-slit experiment in a bit more detail, as well as a similar experiment using particles.

Young's Experiment—One Slit at a Time. Assume as before that a single-frequency plane wave of light, ψ, is incident on the double-slit apparatus, as shown in Fig. 2.4. However, this time we will consider what happens when only one slit is open.

If first only slit 1 is open, the intensity pattern $I_1 = |\psi_1|^2$ is seen on the screen, as shown in the figure. In a similar manner, if only slit 2 is open, then $I_2 = |\psi_2|^2$. However, if both slits are open, we obtain the (interference) intensity pattern $I = |\psi_1 + \psi_2|^2$ shown previously in Fig. 2.3, which is not the same as $I_1 + I_2$. Note that, in general,

$$|\psi_1|^2 + |\psi_2|^2 \neq |\psi_1 + \psi_2|^2 = |\psi_1|^2 + |\psi_2|^2 + 2Re\left(\psi_1^* \psi_2\right), \tag{2.11}$$

where ψ^* is the complex conjugate of ψ and $Re\,(z)$ indicates that we take the real part of the complex quantity z. Thus, when the absolute value of the wavefunction is taken, its phase information is lost. Therefore, since interference effects are a result of phase differences of

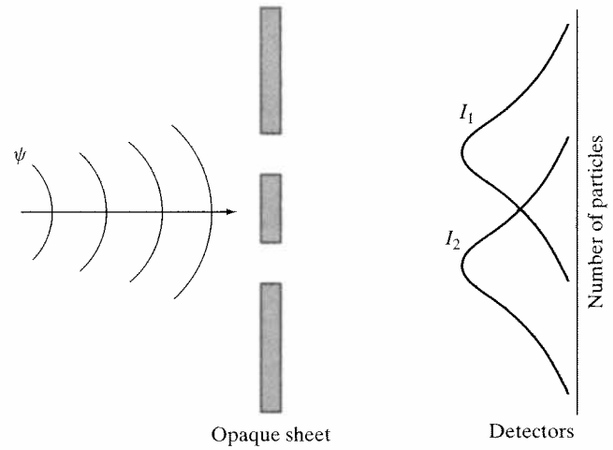


Figure 2.4 Modification of Young's double-slit experiment, when only one slit is open. Intensity pattern I_1 results when slit 1 (the top slit) is open and slit 2 (the bottom slit) is closed, and intensity pattern I_2 results when slit 1 is closed and slit 2 is open.

the two waves involved, ψ_1 and ψ_2 need to be added together before taking the absolute value to obtain the correct result.[†] So far, all seems well.

Young's Experiment—What to Expect with Classical Particles. Now consider the same experiment, but with classical particles. On the far left of the two slits, a source fires particles at the slits in varying directions, but with the same energy. The screen is now an array of closely spaced particle detectors, and the intensity of the particle beam at any point along the screen will be the number of particles arriving at that point per second. The situation is depicted in Fig. 2.5.

When only one of the slits is open, the intensity pattern I_1 or I_2 is obtained, which resembles those obtained in the similar wave experiment of Fig. 2.4. If both slits are open simultaneously, for classical particles we expect that the intensity pattern is merely $I_1 + I_2$, as shown by the dashed line in Fig. 2.5, since each particle moves along a certain trajectory, either through one slit or the other (or bouncing backwards if they weren't heading for a slit). The fact that either one slit, or both slits, are open makes no difference to any given particle.

The particle beam can be sufficiently sparse, such that only one particle is passing through the slits at any given time, so that they don't interfere (collide) with each other. Again, so far, all seems well.

Young's Experiment and the Concept of Photons—One More Time with Light, but Slowly. Armed with this knowledge, we now reconsider the double-slit experiment with light. Rather than simply watching for bright and dark spots on a screen placed

[†] As a simple example, consider two plane waves $\psi_1 = e^{ikz}$ and $\psi_2 = e^{-ikz}$. Then, $|\psi_1 + \psi_2| = 2\,|\cos(kz)|$, showing constructive and destructive interference at certain points z. However, $|\psi_1| + |\psi_2| = 1 + 1 = 2$, independent of position.

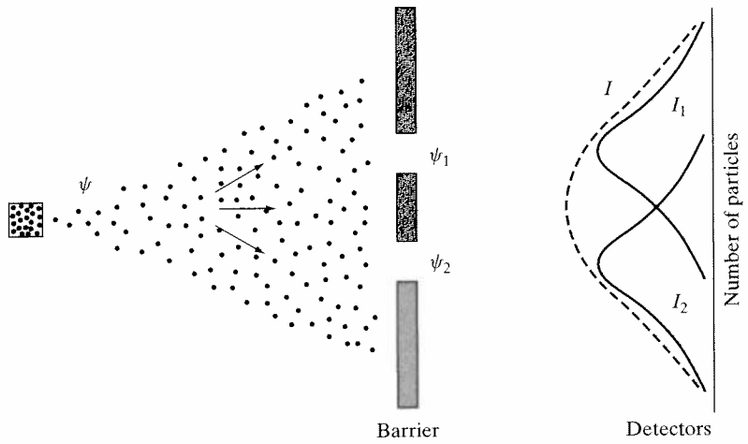


Figure 2.5 Young's double-slit experiment involving classical particles. When one slit is open the individual intensity pattern I_1 or I_2 is obtained. When both slits are simultaneously open, the intensity pattern $I = I_1 + I_2$ results, shown as the dashed line.

behind the slits, we use optical detectors that register the presence of optical energy. With only slit 1 open, we reduce the intensity of the incoming light. If the intensity is reduced enough, so that only one detector is active at any time, we would find that energy is not arriving continuously, but in discrete bursts, pointing to a particle-like nature of light. (It is only because these energy bundles are usually arriving at such a fast rate that we ordinarily don't notice their discrete nature.)

A few years before Lenard's experiment on the energy of photo-emitted electrons, Max Planck had satisfactorily explained blackbody radiation by proposing that the energy emitted by a blackbody should be quantized (i.e., energy should occur in discrete units), such that

$$E = hf = \hbar\omega, \tag{2.12}$$

where h is a constant (now called *Planck's constant*) and f is frequency (ω is radian frequency, $\omega = 2\pi f$), where

$$\hbar = h/2\pi, \tag{2.13}$$

$$h = 6.6261 \times 10^{-34} \text{ Js},$$

$$\hbar = 1.0546 \times 10^{-34} \text{ Js}.$$

In 1905, Albert Einstein explained the photoelectric effect by applying Planck's quantization to all electromagnetic waves, and describing for the first time what is now called a *photon*.

It is interesting that Einstein won the 1921 Nobel prize in physics for his explanation of the photoelectric effect, and not for his theory of relativity, which he also proposed in 1905.

So the discrete nature of light is now recognized as quantized electromagnetics waves, called photons. For the photon single-slit experiment using very low-intensity light (i.e., a very sparse photon stream), over time the intensity pattern I_1 shown in Fig. 2.4 will emerge. We are back to something of a particle theory of light.

Young's Experiment—A Very Strange Result Concerning Interference. Now let both slits be open, and use a light intensity that is so low that only one photon is present at any given time (as in the classical particle experiment). Recording the detector output over time, if photons behaved as classical particles, the resulting intensity pattern should be simply $I_1 + I_2$, the result expected for classical particles shown in Fig. 2.5. Instead, we find that the resulting intensity pattern shows interference effects, depicted in Fig. 2.3, and that the observed pattern corresponds to the pattern expected based on a wave theory! This observation shows that photons are not classical particles. The photons pass through the slits *individually*, but somehow interfere *with themselves* in the process. This is a fairly bad situation, to be sure, from the point of view of understanding light in terms of everyday experiences.

Perhaps the most disturbing thing to consider is that at a point where the interference pattern has a minimum, more photons will arrive at that spot with only one slit open than if both slits are open at the same time. Since the intensity is so low that only one photon is present at a time, opening an additional pathway to the detectors could not possibly reduce the number of photons arriving at a certain spot, if photons were really particles. So we are left with a view that light exhibits wave-like and particle-like behavior, but is clearly *neither* a classical wave nor a classical particle—we call this a *quantum particle*. In a sense, one must accept that light is "its own thing"; light has the properties of, well, light. That is, light[†] does not have an analogous counterpart to an everyday, familiar object, which makes its interpretation somewhat difficult and unsatisfying. However, it often suffices to know the properties of light, as partially described in the preceding discussion, in order to interpret experiments and predict behavior.

2.4 ELECTRONS AS PARTICLES, ELECTRONS AS WAVES

2.4.1 Electrons as Particles—The Early Years

Although the concept of electrical charge has been around for most of recorded history, it was only in the early 1800s that the existence of atoms was first established. It was, at first, generally thought that an atom was an indivisible particle. The concept of the electron, as a constituent of an atom, was first developed in the late 1800s, due to experiments by

[†]Recall that all electromagnetic energy (radio waves, light, X-rays, etc.) is the same phenomenon, it is only a matter of different frequencies of oscillation.

John Joseph (J. J.) Thomson. Shortly after, in the early 1900s, Robert Millikan measured the charge of an electron. Therefore, the concept of the electron was fairly new at the time that the photoelectric effect was puzzling scientists.

As the concepts of electrons and atomic structure came about, electrons were naturally thought to be simply very small charged particles. One of the early successes of this model was the prediction of the conductivity of metals, the so-called free *electron gas model.*[†] In fact, this classical model will be used to some degree later on. However, the quantization of light led to the possibility of other phenomena being quantized.

2.4.2 A Little Later—Electrons (and Everything Else) as Quantum Particles

The fact that light is made up of photons lead Louis de Broglie in 1923 to make the radical suggestion that all "particles" having energy E and momentum p should have wavelike properties, too. He proposed that associated with each particle of momentum p is a wave having wavelength (now called the *de Broglie wavelength*)

$$\lambda = \frac{h}{p}, \tag{2.14}$$

so that

$$p = \hbar\frac{2\pi}{\lambda} = \hbar k, \tag{2.15}$$

where k is the wavenumber. When applied to matter, like electrons, these waves are called *matter waves*. De Broglie's prediction was verified for electrons (somewhat accidentally) by Clinton Davission and Lester Germer in 1926 to 1927 using crystal diffraction (not double-slit) techniques. In fact, although double-slit-like experiments with electrons have long been discussed, their successful implementation, using one electron at a time, did not occur until the 1970s. These experiments were repeated with more accuracy in the 1980s. Figure 2.6 shows an experimental demonstration of electron diffraction interference effects using a very sparse stream of electrons. Frames (a)–(d) represent detected electrons at increasingly later times. At first, the detected pattern of electrons seems random. As time increases, the apparent random distribution of electrons begins to form a clear diffraction pattern, in exactly the same way as discussed previously for photons. Since in the experiments electrons pass through the apparatus one at a time, an electron must clearly interfere with itself.

Note that energy quantization, $E = \hbar\omega$, where E is the total (kinetic plus potential) energy, applies to matter waves as well as photons. Since momentum is really a vector quantity, in general,

$$\mathbf{p} = \hbar\mathbf{k}. \tag{2.16}$$

[†]Ohm's law, which states that for many materials the amount of electrical current passing through the material is proportional to the applied voltage, $I = V/R$, where $1/R$ is the proportionality constant, was discovered much earlier, around 1827.

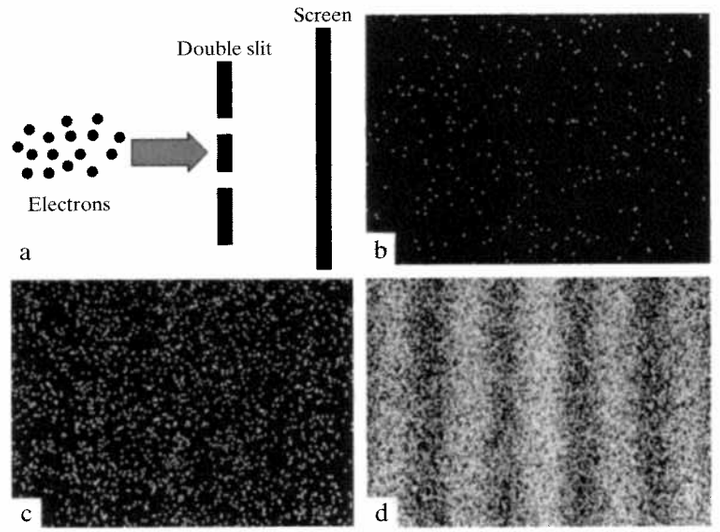


Figure 2.6 Experimental demonstration of interference effects in electron diffraction. Frames (a)–(d) represent increasing time, over which the apparent random distribution of electrons forms a diffraction pattern. (Based on Tonomura, A., et al., "Demonstration of Single-Electron Build-Up of an Interference Pattern," *Am. J. Phys.* 57 (1989): 117. Courtesy of the American Institute of Physics. © Hitachi Ltd. Advanced Research Laboratory.)

The reason we don't see everyday objects behaving as waves is the small numerical value of Planck's constant, given by (2.13). With

$$\lambda = \frac{h}{p} = \frac{h}{mv} \tag{2.17}$$

for objects with mass, it can be seen that, since h is extremely small, m must be very small in order to obtain a wavelength large enough to observe wave-like interactions with physical systems of interest. For example, to see wave effects on the scale of nanometers, we need $\lambda \sim$ nm, which can occur for electrons and other subatomic particles that are extremely light, but generally not for heavier particles. In fact, it is often difficult to observe wave effects for particles heavier than electrons. For example, consider a 1 kg mass moving at 1 m/s. Then, the de Broglie wavelength is

$$\lambda = \frac{h}{p} = \frac{6.6 \times 10^{-34}\ \text{Js}}{(1\ \text{kg})\,(1\ \text{m/s})} = 6.6 \times 10^{-34}\ \frac{\text{Js}^2}{\text{kg m}} = 6.6 \times 10^{-34}\ \text{m}, \tag{2.18}$$

which is much too small to lead to observable wave phenomena.[†] In particular, when λ is small compared to the distance over which potential energy changes, quantum particles

[†]As mentioned previously, wave effects such as diffraction are most easily seen when the wavelength is on the order of, or larger than the characteristic dimensions of the system in question.

behave in a classical manner (i.e., quantum effects are too small to notice). In fact, many aspects of classical physics can be obtained by setting $h = 0$ in the various expressions obtained from quantum theory (note that $h = 0$ decouples energy and frequency). Therefore, the 1 kg mass is far too heavy to be able to observe wave effects, and so it acts like a classical particle. However, if the mass was 10^{-31} kg, then $\lambda = 6.6 \times 10^{-3}$ m, and wave effects would be observable in systems on the scale of millimeters. To date, wave effects have been observed with objects ranging from subatomic particles (e.g., electrons) to relatively heavy 2 nm molecules.

As a comparison, the wavelength of a 1 eV photon is[†]

$$\lambda_p = \frac{hc}{E} = 1.24\ \mu\text{m}, \tag{2.19}$$

since $E = pc$ for photons, whereas the wavelength of a 1 eV electron with only kinetic energy is

$$\lambda_e = \frac{h}{\sqrt{2m_e E}} = 12.3\ \text{Å}. \tag{2.20}$$

Therefore, these different particles "see" different worlds, and, in particular, electrons generally exhibit wave effects at atomic dimensions, whereas photons show wave effects at micron dimensions.

Furthermore, to get an idea of the large number of photons usually present in light, assume a light wave carrying 1 μW of power (W = J/s) at $\lambda = 600$ nm. Then, each photon carries

$$E_p = \hbar\omega = \hbar\pi \times 10^{15}\ \text{J} \tag{2.21}$$

of energy. Let N be the number of photons per second (so the unit of N is 1/s). The sum of all N photons has power

$$P = NE_p\ (1/\text{s})\ (\text{J}) = 1\mu\ \text{J/s},$$

so that

$$N = 3 \times 10^{12} \qquad \text{photons/second}.$$

The granularity of this flow is virtually unobservable. This is usually the case, unless great effort is taken to reduce the intensity, and, hence, the number of photons. This is why the discrete nature of light is not easily observed in everyday situations.

[†]eV is *electron volt*—an electron volt is the energy gained by one electron after moving through a potential difference of one volt. Hence, 1 eV= 1.6×10^{-19} J.

2.4.3 Further Development of Quantum Mechanics

In 1925, Erwin Schrödinger gave a talk on de Broglie's work at a seminar in Zürich, after which Peter Debye commented that "to deal properly with waves one had to have a wave equation." While on a vacation in the Swiss Alps one month later, Schrödinger, seemingly motivated by Debye's comment, worked out what came to be known as wave mechanics. This involved a wavefunction ψ that satisfies a wave equation, now called *Schrödinger's equation*.

At first, Schrödinger did not know what the wavefunction actually was, and referred to it by the rather cryptic name of " mechanical field scalar." He at first thought that electrons were not particles at all, but that their particle-like qualities were merely manifestations of a pure wave phenomena involving wavepackets, which are superpositions of waves. In 1927, around the time of Schrödinger's fourth paper on the new wave mechanics, Max Born hypothesized that for each quantum particle there is an associated wave ψ, Schrödinger's wavefunction, the modulus squared ($|\psi|^2$) of which gives the probability of finding the particle at a certain location.

Therefore, in the double-slit experiment, we have the situation where a sparse stream of photons, each with the same energy and momentum, and, hence, the same probability wavefunction ψ, is directed one at a time towards the slits. The wave ψ of each photon interferes *with itself* in passing through the two slits (you could say that the photon passes through both slits at the same time), such that the probability of finding the photon along the row of detectors forms the observed oscillating interference pattern. Of course, a given photon must hit the detectors at some definite point, and so the interference pattern can't be seen by the arrival of one photon. However, over time, the fact that at some locations the probability of finding a photon is small, and at other locations large, leads to the interference pattern ultimately observed. By de Broglie's result, the same is true for electrons, billiard balls, etc. Thus, in a double-slit experiment involving electrons, the electrons are said to pass simultaneously through both slits.

It should be noted that just before Schrödinger's work, in 1925, Werner Heisenberg developed an approach to quantum theory involving sets of complex numbers. Max Born and Pascual Jordan recognized these sets as matrices, and, together with Heisenberg, reformulated the theory as matrix mechanics. In 1926, Schrödinger showed that his method and the method of matrix mechanics were equivalent. In this text, we use Schrödinger's approach because it is a bit more appealing to scientists who are accustomed to dealing with waves. However, perhaps even more important than his matrix mechanics, in 1927, Heisenberg formulated what is now called the *Heisenberg uncertainty principle*, which states that one cannot simultaneously measure the position and momentum of quantum particles with arbitrary precision. Written mathematically, the Heisenberg uncertainty principle is expressed as

$$\Delta p \Delta x \geq \hbar/2. \tag{2.22}$$

This idea is quite important in quantum theory, and it will be used later.

TABLE 2.1 MASS AND CHARGE OF SOME FERMIONS.

Particle	Mass	Charge
electron	$m_e = 9.1095 \times 10^{-31}$ kg	$q_e = -1.6022 \times 10^{-19}$ C $= -e$
proton	$m_p = 1.6726 \times 10^{-27}$ kg	$e = 1.6022 \times 10^{-19}$ C
neutron	$m_n = 1.6750 \times 10^{-27}$ kg	—

Two other key points of quantum theory remain to be discussed, although their historical origins will only be briefly mentioned here. First, in the mid-1920s, it was found that electrons behave in a magnetic field as if they had angular momentum. This phenomenon was initially attributed to the electron spinning about its own axis, and so this quantity was called *spin*. It was quickly determined that the electron was not, in fact, spinning about its own axis, but that spin was an intrinsic quantity associated with the electron. Spin was found to be quantized in multiples of $\hbar$. Particles with integral (in units of $\hbar$) spin are called *bosons*. (Examples are photons and quantized lattice vibrations called *phonons*.) Particles with half-integral spin are called *fermions*. (Examples are electrons, protons, neutrons, quarks, and neutrinos.)[†] Spin has no classical analogue since, although classical particles can possess angular momentum due to orbital motion, or literal spinning (rotating) about an axis, classical objects do not have any intrinsic spin. The typical advice for students learning quantum physics is to accept spin as just another intrinsic property of an object, and not to become bogged down in trying to envision spin in terms of everyday phenomena.

The other key quantum development, also having no classical analogue, was the *Pauli exclusion principle*, proposed in 1925 by Wolfgang Pauli to account for the observed patterns of light emission from atoms. The exclusion principle was quickly generalized to include all quantum particles with nonintegral values of spin, i.e., fermions.

> The Pauli exclusion principle states that two or more identical fermions cannot occupy the same quantum state.

The importance of this seemingly mild statement cannot be overestimated, as this characteristic of fermions is the basis for understanding most materials, including the development of the periodic table, and characteristic properties of insulators, conductors, and semiconductors.

For later reference, the mass and charge of some fermions are listed in Table 2.1.

2.5 WAVEPACKETS AND UNCERTAINTY

Quantum particles (light, electrons, bowling balls, etc.) can be thought of as, in some sense, quantized bundles of energy $E = \hbar\omega$, having wave-like properties (frequency, ω, and wavelength, λ), and particle-like properties (momentum, p) that are interrelated—the so-called wave–particle duality. For example, electrons have a finite and definite charge and mass (in a nonrelativistic sense, the rest mass), which seems like a particle property, although electrons also have a de Broglie wavelength, and can exhibit wave-like diffraction (usually at atomic length scales). Photons have no mass or charge, but can be thought of as "pure energy." As described previously, photons exhibit both wave-like and particle-like behavior.

One attribute of classical particles is that they have a certain trajectory in moving through space that can be described using Newton's laws. For example, in one dimension, a particle occupies a certain position $x(t)$ at a certain time t. On the other hand, consider a typical plane wave

$$\psi(t, x) = Ae^{-i(\omega t - kx)}, \tag{2.23}$$

in one dimension, where A is the amplitude, ω is the radian frequency, and k is the wavenumber ($k = 2\pi/\lambda$). Wave propagation (classical electromagnetic fields, pressure, displacement, etc.) can often be characterized by a plane wave ψ that extends over a region of (or all of) space, rather than being localized to a single point. The field is a function of position x and time t as independent variables (although k and ω are interrelated). Wave–particle duality would seem to imply that quantum particles will not be localized at a single point, like a classical particle, nor spread out over all space, like a classical plane wave, but will be something in between these two cases. For instance, free electrons in space usually have energies that make the de Broglie wavelength very small, such that diffraction and interference effects can often be ignored. Viewed from a distance large compared to its wavelength, an electron appears like a particle. Viewed from a distance small compared to its wavelength, usually atomic dimensions, the " spread" of the electron becomes evident. At sufficiently low energies the wave nature of the electron becomes evident over larger space scales, since momentum becomes smaller and so, by (2.14), wavelength becomes larger.

One way to model this dual behavior is with a *wavepacket*, which is a wave that is both propagating and localized in space and time. If viewed from a sufficiently large distance (relative to wavelength), the wavepacket looks like a particle moving along some trajectory. Viewed from a sufficiently small distance, one can see the " spread" of the wavepacket. Therefore, the wavepacket has attributes of both waves and particles, which is obviously something that is needed for quantum particles. Although wavepackets won't be used explicitly in the detailed examples later in the text, the basic ideas will be presented here as a conceptual tool. In addition, this leads to the important concepts of phase and group velocity.

To understand wavepackets, one first needs to appreciate some aspects of waves. Consider the single frequency plane wave given by (2.23), and recall that frequency and wavenumber are related, that is, $\omega = \omega(k)$ or $k = k(\omega)$. For example, for a photon, the familiar relationship between velocity, wavelength, and frequency,

$$c = \lambda f, \tag{2.24}$$

[†]Furthermore, any object that is made up of even number of fermions is a (composite) boson, whereas any particle that is made up of an odd number of fermions is a (composite) fermion. Therefore, hydrogen, with one electron and one proton, is a boson. Helium, with two each of electrons, protons, and neutrons, is also a boson.

where c is the speed of light, leads to

$$c = \lambda \frac{\omega}{2\pi} \rightarrow \omega = \frac{2\pi}{\lambda} c = kc,$$

such that

$$\omega(k) = ck. \tag{2.25}$$

For a particle with mass m and only kinetic energy,

$$E = \hbar\omega = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m}, \tag{2.26}$$

such that

$$\omega(k) = \frac{\hbar k^2}{2m}. \tag{2.27}$$

Relationships between frequency and wavenumber such as (2.25) and (2.27) are called *dispersion relations*.

The *phase velocity* of the plane wave (2.23) is the velocity of a constant phase (and amplitude, in this case) planar wavefront. Therefore, setting the phase term equal to a constant C,

$$\omega t - kx = C, \tag{2.28}$$

and differentiating with respect to time leads to[†]

$$\omega - k\frac{dx}{dt} = \omega - kv_p = 0, \tag{2.29}$$

such that the phase velocity is given by

$$v_p = \frac{\omega}{k}. \tag{2.30}$$

For the plane wave (2.23) this is the only idea of velocity. However, (2.23) describes a wave spread out over all space and time. It certainly has wave behavior, but it does not resemble a particle (localized energy bundle).

[†]We said previously that t and x are independent in the wave picture. This is true, in the manner in which they are used in (2.23). However, once we set the phase term $\omega t - kx$ equal to a constant (to "watch" a specific point on the waveform move), then, as t increases, x must increase to keep $\omega t - kx$ constant. Therefore, $x = x(t)$ for purposes of keeping track of the advancement in time of the constant-phase point.

Now, instead of a single plane wave, consider the quantity

$$\psi(x,t) = \int_{-\infty}^{\infty} a(k)\, e^{-i(\omega(k)t - kx)} dk, \tag{2.31}$$

where the dependence $\omega = \omega(k)$ is explicitly included. It should be first noted that for any value of k, $e^{-i(\omega(k)t-kx)}$ is merely a plane wave having wavenumber k and related frequency $\omega = \omega(k)$, and $a(k)$ is just a number, interpreted as the amplitude of the plane wave. Therefore, the integrand of (2.31) represents plane waves of varying amplitudes and wavenumbers, and the integration is simply a summation of those plane waves.

It can be shown that (2.31) can represent a wave localized in space, i.e., a wavepacket (like a bundle of waves). For example, assume

$$\begin{aligned} a(k) &= 1, \quad k_0 - \Delta k \le k \le k_0 + \Delta k, \\ &= 0, \quad \text{elsewhere}, \end{aligned} \tag{2.32}$$

as shown in Fig. 2.7.

With this form for $a(k)$, one can interpret (2.31) as a summation of waves with wavenumbers within some Δk range of a given value k_0. The integral (2.31) becomes

$$\psi(x,t) = \int_{k_0-\Delta k}^{k_0+\Delta k} e^{-i(\omega(k)t - kx)} dk, \tag{2.33}$$

which can't be evaluated unless the dispersion relation $\omega(k)$ is known.

It is useful to consider several simple cases, beginning with the situation, as for photons in free space, where ω is linear in k, $\omega = ck$. Then, (2.33) becomes

$$\psi(x,t) = \int_{k_0-\Delta k}^{k_0+\Delta k} e^{-ik(ct-x)} dk \tag{2.34}$$

$$= 2\Delta k\, e^{-ik_0(ct-x)} \frac{\sin(\Delta k(ct-x))}{\Delta k(ct-x)}, \tag{2.35}$$

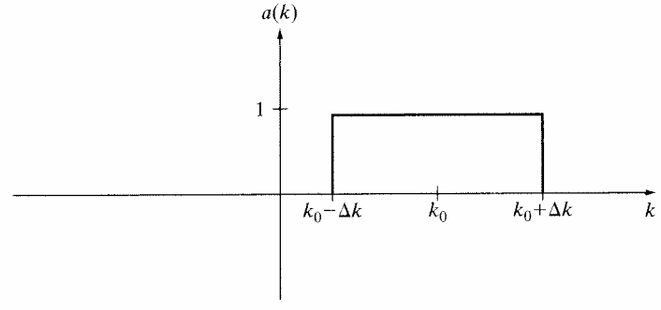


Figure 2.7 Rectangular amplitude distribution for wavepacket construction.

which is a wavepacket moving with velocity c (note that $v_p = \omega/k = c$) and having an envelope proportional to

$$\text{sinc}\left(\Delta k\left(ct - x\right)\right) \equiv \frac{\sin\left(\Delta k\left(ct - x\right)\right)}{\Delta k\left(ct - x\right)}. \tag{2.36}$$

The function $\text{sinc}(x) = \sin(x)/x$ is centered at $x = 0$ and decays away from that point, as shown in Fig. 2.8.

Therefore, the wavepacket (2.35) is concentrated around the point $x = ct$ at a given time t, and moves at the phase velocity $v_p = c$. Referring to the discussion of quantum particles, it seems reasonable to model a quantum particle as being associated with a wavepacket, since a wavepacket exhibits wave-like behavior and, when viewed from a distance large compared to the spread of the envelope (the sinc function), it resembles a particle, since it is somewhat localized in space.

As an interesting aside, the behavior of the sinc function can be used to gain insight into the Heisenberg uncertainty principle. Consider the function $\text{sinc}(\Delta k x)$. If the spread in wavenumbers Δk is very small, then, since $p = \hbar k$, the momentum varies over a small range. Due to the argument of the sinc function, the wavepacket envelope is spread out over a large range of space, x. So a small spread in momentum indicates a large spread in position. As Δk increases, the wavepacket will become more concentrated in space.

In particular, the function $\text{sinc}(\Delta k x)$ is rapidly decreasing outside some range Δx centered at $x = 0$, and one can consider the wave to be "contained" within this region of space. It is useful to choose the width of the wavepacket in space to extend to the points where the amplitude of the wavepacket's envelope decreases to 63 percent of its initial value. That is, the spatial extent of the wavepacket is described by Δx such that

$$\Delta k \Delta x = \frac{\pi}{2}. \tag{2.37}$$

Of course, this choice is somewhat arbitrary, but is one of many reasonable choices. The relation (2.37) makes it clear that increasing Δk causes Δx to decrease, and vice versa.

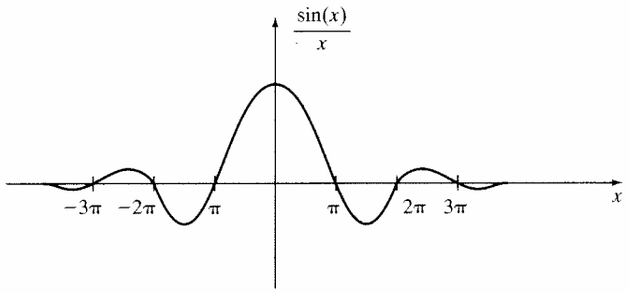


Figure 2.8 Plot of $\sin(x)/x$ versus x.

Therefore, a wavepacket tightly confined in space is made up of plane waves having a large spread in wavenumbers, and a wavepacket loosely confined in space is made up of plane waves having a small spread in wavenumbers.

If Δk goes to zero, then the wavenumber (and momentum) is known exactly, and then Δx must go to infinity to maintain (2.37), so that the position can be any value. If Δx goes to zero, then the position is known exactly, and, conversely, Δk must go to infinity, so that momentum can take any value. Using $k = p/\hbar$, one obtains

$$\Delta p \Delta x = \frac{\hbar \pi}{2}, \tag{2.38}$$

which, except for the factor of π, is almost the famous Heisenberg uncertainty principle,

$$\Delta p \Delta x \geq \hbar/2. \tag{2.39}$$

The uncertainty principle states that we cannot know both momentum and position to arbitrary accuracy. If we know the position of a particle with great precision (Δx small), then the uncertainty in the particle's velocity is very large. Therefore, since the Heisenberg uncertainty principle applies to quantum particles, and is at least qualitatively consistent with the idea of a wavepacket, we can have some confidence in thinking of quantum particles as wavepackets.

As an example, consider an electron. If we know the position of an electron to nanoscale accuracy, $\Delta x = 10^{-9}$ m, then, from (2.39), $\Delta p \geq 5.25 \times 10^{-25}$ kg m/s, and $\Delta v = \Delta p/m_e \geq 5.77 \times 10^5$ m/s, which is a large uncertainty in the electron's velocity. Thus, as expected, at atomic dimensions, the quantum nature of the particle is very important.

If we instead consider a macroscopic object such as a paper clip, the situation is quite different. Assume that we know the position of a paper clip to within 1 mm (10^{-3} m), a reasonable assumption since, perhaps, it is sitting on a table in front of us. Assume that the paper clip has mass 10^{-3} kg. Then, the uncertainty in the paper clip's velocity is

$$\Delta v \geq \frac{\hbar/2}{m\Delta x} = \frac{1.05 \times 10^{-34}}{(2)\,10^{-3}10^{-3}} = 5.25 \times 10^{-29} \text{ m/s}, \tag{2.40}$$

which is an extremely small number. Our everyday intuition would lead us to believe that the paper clip is stationary, i.e., that $v = 0$. However, at 5.25×10^{-29} m/s, it would take 1.9×10^{22} seconds (about 6×10^{14} years) for the paper clip to move just 1 μm. Recent observations from the Hubble Space Telescope indicate that the age of the universe is around 14 billion years, which is 14×10^9 years! Thus, there is no way for us to say that the paper clip sitting on the table in front of us is not really moving, albeit extremely slowly. Thus, the Heisenberg uncertainty principle applies to all objects,

but for familiar macroscopic objects, it leads to results that are consistent with everyday observations.

Notice that the uncertainty principle (2.39) is for a one-dimensional system, and therefore one can say that it relates momentum in the x-coordinate and position along the x-coordinate, i.e.,

$$\Delta p_x \Delta x \geq \hbar/2. \tag{2.41}$$

Generalizing to three dimensions, we have

$$\Delta p_x \Delta x \geq \hbar/2, \tag{2.42}$$

$$\Delta p_y \Delta y \geq \hbar/2, \tag{2.43}$$

$$\Delta p_z \Delta z \geq \hbar/2, \tag{2.44}$$

so that the uncertainty principle does not preclude the simultaneous measurement of, say, momentum p_x and position z. This will be discussed further in Section 3.1.4.

One can gain an intuitive understanding of the position-momentum uncertainty principle for a quantum particle by the following reasoning. If one measures, say, the position of a macroscopic object by shining light on it, the momentum carried by the illuminating photons will not measurably change the momentum of the object, due to its large mass. Thus, the object's position can be measured without changing its momentum. However, this is not the case for an atomic or subatomic particle, due to its extremely small mass.

From (2.39), one can obtain an uncertainty relationship between energy and time. Using $p = \hbar k$, $E = \hbar\omega$, and, specifically for photons, $k = \omega/c$ and $c\Delta t = \Delta x$, then

$$\Delta E \Delta t \geq \hbar/2. \tag{2.45}$$

Although (2.45) was obtained from the quantum uncertainty between momentum and position, it is really a classical uncertainty between time-frequency Fourier transform quantities (i.e., using $E = \hbar\omega$, we obtain $\Delta\omega\Delta t \geq 1/2$).

Dispersion. Returning to the discussion of wavepackets, we find that in the case considered previously, the wavepacket does not change its shape as it propagates. Often, as will be seen in later chapters, one needs to consider a dispersion relation that is more complicated than the simple linear dependence considered above for photons in free space. In general, this leads to the wavepacket changing shape (generally, spreading out) as it propagates. In addition, in this case the phase velocity is not the velocity of primary interest.

To examine this phenomenon, it is convenient to expand $\omega(k)$ in a Taylor's series around the center wavenumber $k = k_0$, obtaining

$$\begin{aligned}\omega(k) &= \omega(k_0) + \left.\frac{\partial\omega}{\partial k}\right|_{k=k_0}(k-k_0) + \frac{1}{2}\left.\frac{\partial^2\omega}{\partial k^2}\right|_{k=k_0}(k-k_0)^2 + \ldots \\ &= \omega_0 + \alpha(k-k_0) + \beta(k-k_0)^2 + \ldots.\end{aligned} \tag{2.46}$$

Now assume that it is sufficient to keep only the first two terms in (2.46). Then,

$$\begin{aligned}\psi(x,t) &\simeq e^{-ik_0(v_p t - x)} \int_{k_0-\Delta k}^{k_0+\Delta k} e^{-i(k-k_0)(\alpha t - x)} dk \\ &= e^{-ik_0(v_p t - x)} 2\Delta k \frac{\sin(\Delta k(\alpha t - x))}{\Delta k(\alpha t - x)},\end{aligned} \tag{2.47}$$

where $v_p = \omega_0/k_0$. The velocity of the envelope is not the phase velocity, but α,

$$\alpha = \left.\frac{\partial\omega}{\partial k}\right|_{k=k_0} = v_g, \tag{2.48}$$

which is called the *group velocity*. Therefore,

$$\psi(x,t) \simeq e^{-ik_0(v_p t - x)} 2\Delta k \frac{\sin(\Delta k(v_g t - x))}{\Delta k(v_g t - x)}. \tag{2.49}$$

In this case, the wavepacket moves through space and time as a localized bundle of approximate width

$$\Delta k(v_g t - x) = \frac{\pi}{2} \tag{2.50}$$

that is centered at the point

$$(v_g t - x) = 0. \tag{2.51}$$

That is, starting at $t = 0$, the wavepacket is centered at $x = 0$, and at a given time t the wavepacket is centered at the point

$$x = v_g t \tag{2.52}$$

and occupies a spatial extent

$$\Delta x = v_g t - \frac{\pi}{2\Delta k}. \tag{2.53}$$

As mentioned above, the group velocity is the velocity of the wavepacket's envelope, rather than the phase velocity of the " center" plane wave that has wavenumber k_0. The phase velocity being associated with the center plane wave is a result of the approximate expansion of the $\omega(k)$ relationship. The wavepacket is actually made up of planes waves, each with an individual wavenumber k and associated phase velocity $v_p = \omega/k$. Each different plane wave moves at a different velocity. Over time, the plane waves will reach a given point at different times, tending to spread out the wavepacket's envelope, the width of which, according to (2.53), grows as time increases. So the center of the wavepacket moves as time changes, indicating propagation (or a particle trajectory), and the wavepacket simultaneously spreads out in space as time increases.

It should be noted that often, rather than the abrupt amplitude function $a(k)$ given by (2.32), a more physically realistic function is used, typically a Gaussian,

$$a(k) = e^{-\frac{(k-k_0)^2}{2\Delta k^2}}. \tag{2.54}$$

However, in this case, the calculations shown previously become a bit more complex than for the simple function (2.32).

2.6 MAIN POINTS

This chapter presented some information on the origins of quantum theory, and compared classical physics and, in particular, classical particles and waves, with quantum physics. After reading this chapter, you should know that

- classical particles have a definite position in space, and definite velocity and momentum;
- quantum mechanics states that we can only know the probability of a particle being at a certain position at a certain time, and that it is impossible to measure precisely both the position and momentum of a particle;
- quantum mechanics arose from experiments in the later 1800s and early 1900s concerning thermal blackbody radiation and the photoelectric effect that could not be explained by classical physics;
- in the quantum picture, energy is quantized as $E = \hbar\omega$;
- all "particles" having energy and momentum have wave-like properties, described by the de Broglie wavelength. When the material space in question is large compared to λ, the particle acts like a classical particle. When the space is small compared to λ, the particle exhibits wave-like properties.

Furthermore, you should

- be familiar with the idea of spin, and the Pauli exclusion principle;
- know what fermions and bosons are, and their relationship to the exclusion principle;
- understand wavepacket concepts, and the idea of phase and group velocity.

2.7 PROBLEMS

1. What is the energy (in J and eV) of a photon having wavelength 650 nm? Repeat for an electron having the same wavelength and only kinetic energy.

2. For light (photons), in classical physics the relation

$$c = \lambda f \tag{2.55}$$

is often used, where c is the speed of light, f is the frequency, and λ is the wavelength. For photons, is the de Broglie wavelength the same as the wavelength in (2.55)? Explain your reasoning. Hint: Use Einstein's formula

$$E = mc^2 = \sqrt{p^2c^2 + m_0c^4}, \tag{2.56}$$

where m_0 is the particle's rest mass, which, for a photon, is zero.

3. Common household electricity in the United States is 60 Hz, a typical microwave oven operates at 2.4×10^9 Hz, and UV light occurs at 30×10^{15} Hz. In each case, determine the energy of the associated photons in J and eV.

4. Assume that a HeNe laser pointer outputs 1 mW of power at 632 nm.

(a) Determine the energy per photon.
(b) Determine the number of photons per second, N.

5. Repeat Problem 2.4 if the laser outputs 10 mW of power. How does the number of photons per second scale with power?

6. Calculate the de Broglie wavelength of

(a) a proton moving at 437, 000 m/s
(b) a proton with kinetic energy 1,100 eV
(c) an electron traveling at 10,000 m/s
(d) an 800 kg car moving at 60 km/h

7. Determine the wavelength of a 150 g baseball traveling 90 m/h. Use this result to explain why baseballs do not seem to diffract around baseball bats.

8. How much would the mass of a ball need to be in order for it to have a de Broglie wavelength of 1 m (at which point its wave properties would be clearly observable)? Assume that the ball is traveling 90 m/h.

9. Determine the momentum carried by a 640 nm photon. Since a photon is massless, does this momentum have the same meaning as the momentum carried by a particle with mass?

10. Consider a 4 eV electron, a 4 eV proton, and a 4 eV photon. For each, compute the de Broglie wavelength, the frequency, and the momentum.

11. Determine the de Broglie wavelength of an electron that has been accelerated from rest through a potential difference of 1.5 V.

12. Calculate the uncertainty in velocity of a 1 kg ball confined to

(a) a length of 20 μm
(b) a length of 20 cm
(c) a length of 20 m

(d) What can you conclude about observing "quantum effects" using 1 kg balls? What kind of objects would you need to use to see quantum effects on these length scales?

13. If we know that the velocity of an electron is 40.23 ± 0.01 m/s, what is the minimum uncertainty in its position? Repeat for a 150 g baseball traveling at the same velocity.

14. If a molecule having mass 2.3×10^{-26} kg is confined to a region 200 nm in length, what is the minimum uncertainty in the molecule's velocity?

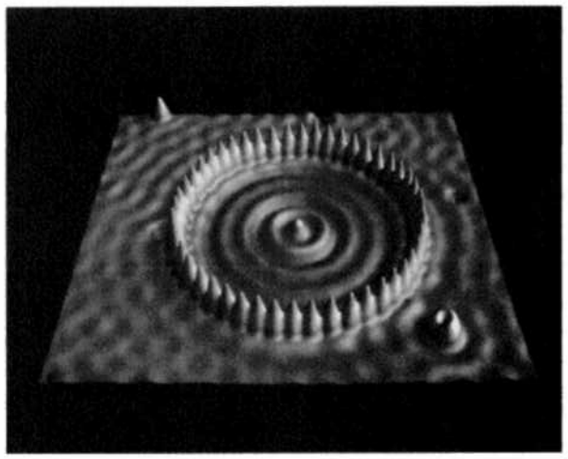
15. Determine the minimum uncertainty in the velocity of an electron that has its position specified to within 10 nm.

16. Explain the difference between a fermion and a boson, and give two examples of each.

Chapter

3

QUANTUM MECHANICS OF ELECTRONS



STM image of atoms forming a "quantum corral," resulting in standing electron waves. The diameter of the ring is approximately 14 nm. (Courtesy Almaden Research Center/Research Division/NASA/Media Services.)

As described in the previous chapter, in the early 1900s, it became clear that classical Newtonian mechanics was unable to explain a considerable amount of experimentally observed phenomena. Light was recognized to have a discrete nature, and both light and matter were found to exhibit properties of classical waves and classical particles, and, in addition, to exhibit behavior that was completely unknown to classical physics. In the following discussion, when particles (usually electrons, but perhaps atoms, paper clips, billiard balls, etc.) are referred to, it should be recognized that all such objects, irrespective of size, are really quantum particles. The mathematical description of such particles is given by solutions of Schrödinger's equation.[†]

[†]Schrödinger's equation describes quantum particles having mass. Photons, which do not have mass, obey a quantized version of Maxwell's equations, although we will not consider that development here.