CHAPTER

3

Elementary Quantum Physics

The triumph of modern physics is the triumph of quantum mechanics. Even the simplest experimental observation that the resistivity of a metal depends linearly on the temperature can only be explained by quantum physics, simply because we must take the mean speed of the conduction electrons to be nearly independent of temperature. The modern definitions of voltage and ohm, adopted in January 1990 and now part of the IEEE standards, are based on Josephson and quantum Hall effects, both of which are quantum mechanical phenomena.

One of the most important discoveries in physics has been the wave–particle duality of nature. The electron, which we have so far considered to be a particle and hence to be obeying Newton's second law ($F = ma$), can also exhibit wave-like properties quite contrary to our intuition. An electron beam can give rise to diffraction patterns and interference fringes, just like a light wave. Interference and diffraction phenomena displayed by light can only be explained by treating light as an electromagnetic wave. But light can also exhibit particle-like properties in which it behaves as if it were a stream of discrete entities ("photons"), each carrying a linear momentum and each interacting discretely with electrons in matter (just like a particle colliding with another particle).

3.1 PHOTONS

3.1.1 LIGHT AS A WAVE

In introductory physics courses, light is considered to be a wave. Indeed, such phenomena as interference, diffraction, refraction, and reflection can all be explained by the theory of waves. In all these phenomena, a ray of light is considered to be an **electromagnetic (EM) wave** with a given frequency, as depicted in Figure 3.1. The electric and magnetic fields, $\mathcal{E}_y$ and B_z, of this wave are perpendicular to each other and to the direction of propagation x. The electric field $\mathcal{E}_y$ at position x at time t may be

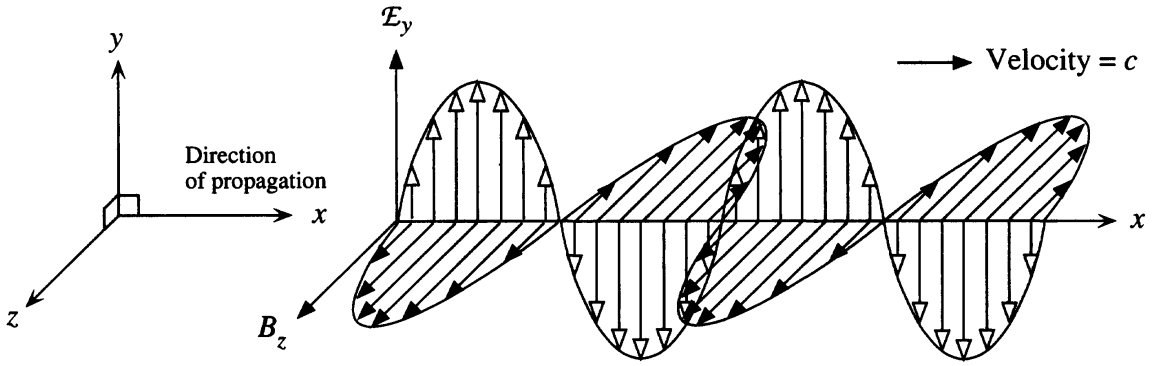


Figure 3.1 The classical view of light as an electromagnetic wave.
An electromagnetic wave is a traveling wave with time-varying electric and magnetic fields that are perpendicular to each other and to the direction of propagation.

described by

Traveling wave

$$\mathcal{E}_y(x, t) = \mathcal{E}_o \sin(kx - \omega t) \qquad [3.1]$$

where k is the wavenumber (propagation constant) related to the wavelength λ by $k = 2\pi/\lambda$, and ω is the angular frequency of the wave (or $2\pi\nu$, where ν is the frequency). A similar equation describes the variation of the magnetic field B_z (directed along z) with x at any time t. Equation 3.1 represents a traveling wave in the x direction, which, in the present example, is a sinusoidally varying function (Figure 3.1). The velocity of the wave (strictly the phase velocity) is

$$c = \frac{\omega}{k} = \nu\lambda$$

where ν is the frequency. The intensity I, that is, the energy flowing per unit area per second, of the wave represented by Equation 3.1 is given by

Intensity of light wave

$$I = \frac{1}{2} c\varepsilon_o \mathcal{E}_o^2 \qquad [3.2]$$

where ε_o is the absolute permittivity.

Understanding the wave nature of light is fundamental to understanding interference and diffraction, two phenomena that we experience with sound waves almost on a daily basis. Figure 3.2 illustrates how the interference of secondary waves from the two slits S_1 and S_2 gives rise to the dark and bright fringes (called **Young's fringes**) on a screen placed at some distance from the slits. At point P on the screen, the waves emanating from S_1 and S_2 interfere constructively, if they are in phase. This is the case if the path difference between the two rays is an integer multiple of the wavelength λ, or

$$S_1P - S_2P = n\lambda$$

where n is an integer. If the two waves are out of phase by a path difference of $\lambda/2$, or

$$S_1P - S_2P = \left(n + \frac{1}{2}\right)\lambda$$

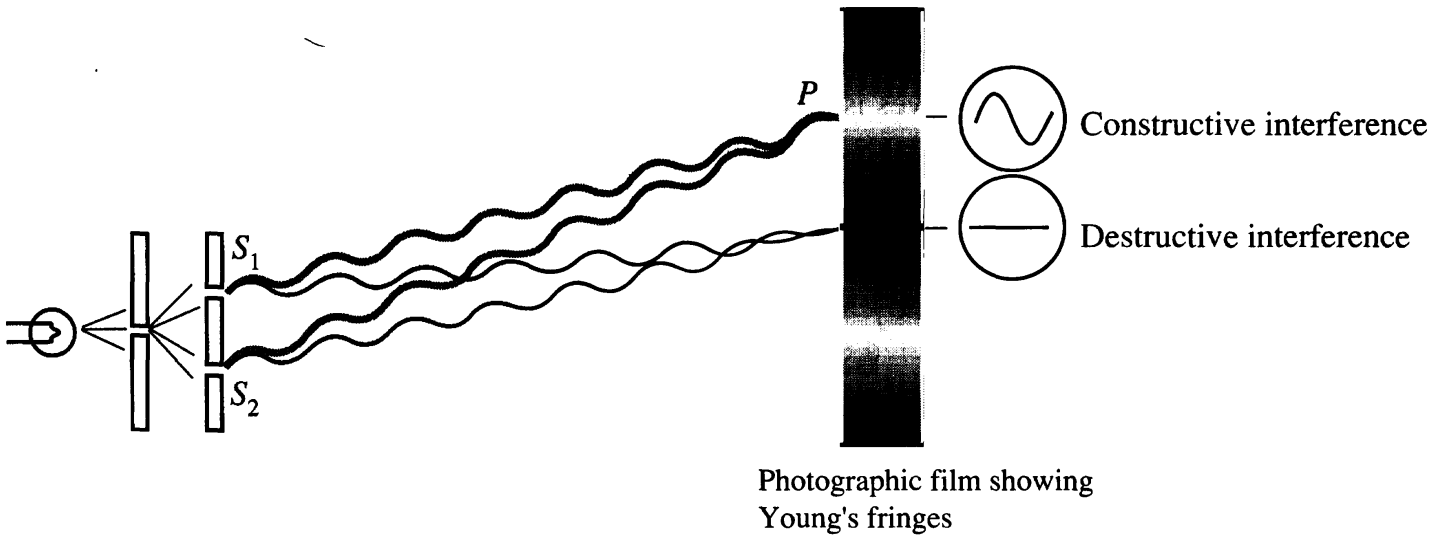


Figure 3.2 Schematic illustration of Young's double-slit experiment.

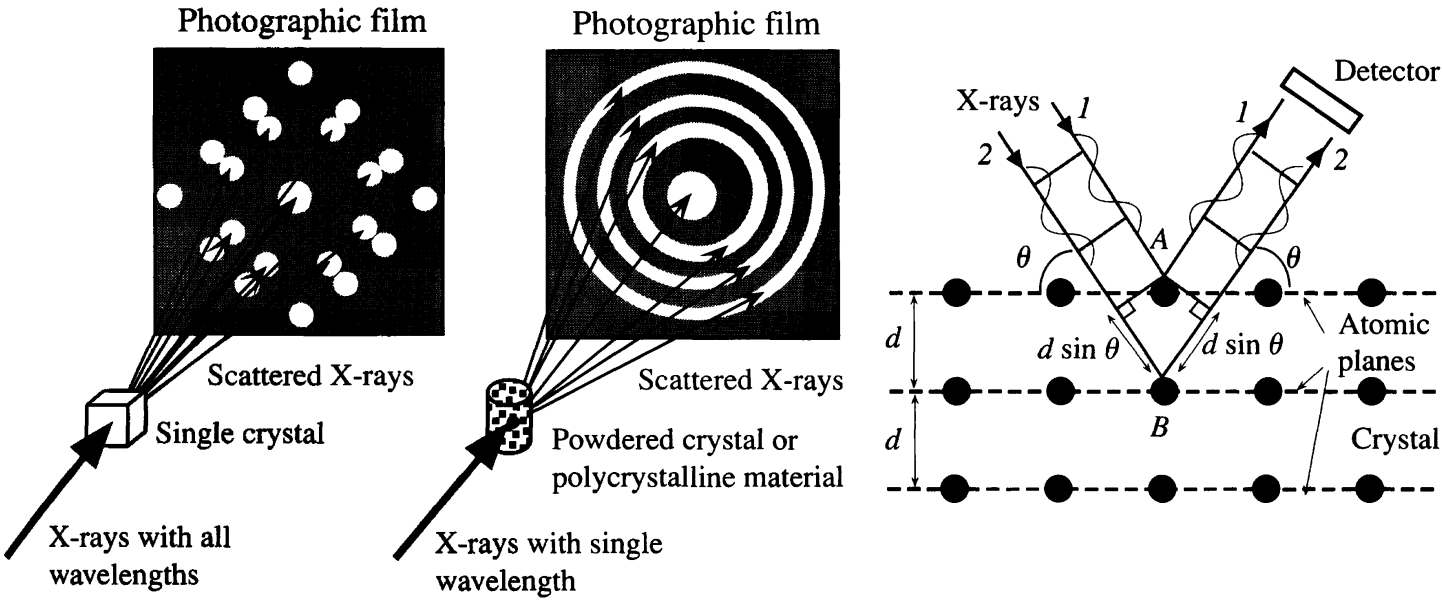


Figure 3.3 Diffraction patterns obtained by passing X-rays through crystals can only be explained by using ideas based on the interference of waves.

(a) Diffraction of X-rays from a single crystal gives a diffraction pattern of bright spots on a photographic film.

(b) Diffraction of X-rays from a powdered crystalline material or a polycrystalline material gives a diffraction pattern of bright rings on a photographic film.

(c) X-ray diffraction involves the constructive interference of waves being "reflected" by various atomic planes in the crystal.

then the waves interfere destructively and the intensity at point P vanishes. Thus, in the y direction, the observer sees a pattern of bright and dark fringes.

When X-rays are incident on a crystalline material, they give rise to typical diffraction patterns on a photographic plate, as shown in Figure 3.3a and b, which can only be explained by using wave concepts. For simplicity, consider two waves, *1* and *2*, in an X-ray beam. The waves are initially in phase, as shown in Figure 3.3c. Suppose that wave *1* is "reflected" from the first plane of atoms in the crystal, whereas

wave 2 is "reflected" from the second plane.[1] After reflection, wave 2 has traveled an additional distance equivalent to $2d \sin\theta$ before reaching wave 1. The path difference between the two waves is $2d \sin\theta$, where d is the separation of the atomic planes. For constructive interference, this must be $n\lambda$, where n is an integer. Otherwise, waves 1 and 2 will interfere destructively and will cancel each other. Waves reflected from adjacent atomic planes interfere constructively to constitute a diffracted beam *only* when the path difference between the waves is an integer multiple of the wavelength, and this will only be the case for certain directions. Therefore the *condition* for the existence of a diffracted beam is

Bragg diffraction condition

$$2d \sin\theta = n\lambda \qquad n = 1, 2, 3, \ldots \qquad [3.3]$$

The condition expressed in Equation 3.3, for observing a diffracted beam, forms the whole basis for identifying and studying various crystal structures (the science of crystallography). The equation is referred to as **Bragg's law,** and arises from the constructive interference of waves.

Aside from exhibiting wave-like properties, light can behave like a stream of "particles" of zero rest-mass. As it turns out, the only way to explain a vast number of experiments is to view light as a stream of discrete entities or energy packets called **photons,** each carrying a quantum of energy $h\nu$, and momentum h/λ, where h is a universal constant that can be determined experimentally, and ν is the frequency of light. This photonic view of light is drastically different than the simple wave picture and must be examined closely to understand its origin.

3.1.2 THE PHOTOELECTRIC EFFECT

Consider a quartz glass vacuum tube with two metal electrodes, a photocathode and an anode, which are connected externally to a voltage supply V (variable and reversible) via an ammeter, as schematically illustrated in Figure 3.4. When the cathode is illuminated with light, if the frequency ν of the light is greater than a certain critical value ν_0, the ammeter registers a current I, even when the anode voltage is zero (*i.e.*, the supply is bypassed). When light strikes the cathode, electrons are emitted with sufficient kinetic energy to reach the opposite electrode. Applying a positive voltage to the anode helps to collect more of the electrons and thus increases the current, until it saturates because all the photoemitted electrons have been collected. The current, then, is limited by the rate of supply of photoemitted electrons. If, on the other hand, we apply a negative voltage to the anode, we can "push" back the photoemitted electrons and hence reduce the current I. Figure 3.5a shows the dependence of the photocurrent on the anode voltage, for one particular frequency of light.

Recall that when an electron traverses a voltage difference V, its potential energy changes by eV (potential difference is defined as work done per unit charge). When a negative voltage is applied to the anode, the electron has to do work to get to this electrode, and this work comes from its kinetic energy just after photoemission. When the negative anode voltage V is equal to V_0, which just "extinguishes" the current I, we

[1] Strictly, one must consider the scattering of waves from the electrons in individual atoms (*e.g.*, atoms *A* and *B* in Figure 3.3c) and examine the constructive interference of these scattered waves, which leads to the same condition as that derived in Equation 3.3.

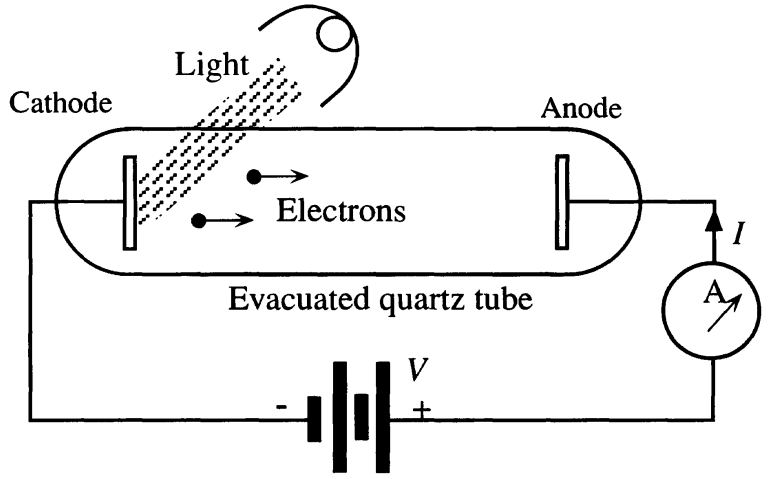
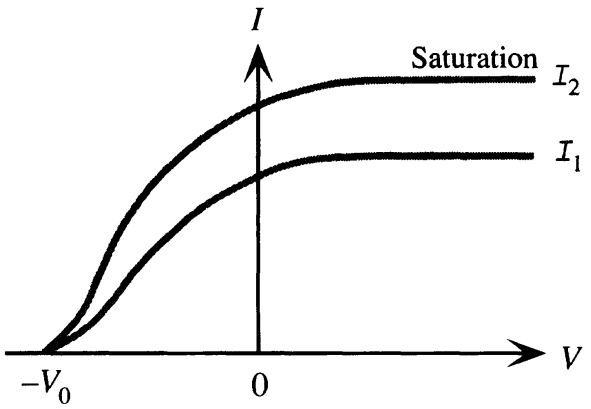
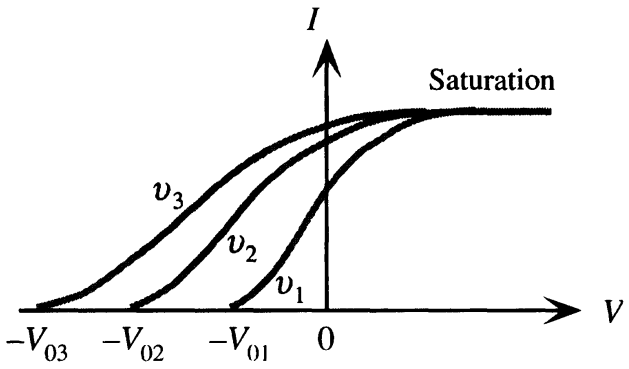


Figure 3.4 The photoelectric effect.



(a) Photoelectric current versus voltage when the cathode is illuminated with light of identical wavelength but different intensities (I). The saturation current is proportional to the light intensity.



(b) The stopping voltage and therefore the maximum kinetic energy of the emitted electron increases with the frequency of light, υ. (The light intensity is not the same; it is adjusted to keep the saturation current the same.)

Figure 3.5 Results from the photoelectric experiment.

know that the potential energy "gained" by the electron is just the kinetic energy lost by the electron, or

$$eV_0 = \frac{1}{2}m_e v^2 = KE_m$$

where v is the velocity and KE_m is the kinetic energy of the electron just after photoemission. Therefore, we can conveniently measure the maximum kinetic energy KE_m of the emitted electrons.

For a given frequency of light, increasing the intensity of light I requires the *same* voltage V_0 to extinguish the current; that is, the KE_m of emitted electrons is independent of the light intensity I. This is quite surprising. However, increasing the intensity does increase the saturation current. Both of these effects are noted in the I–V results shown in Figure 3.5a.

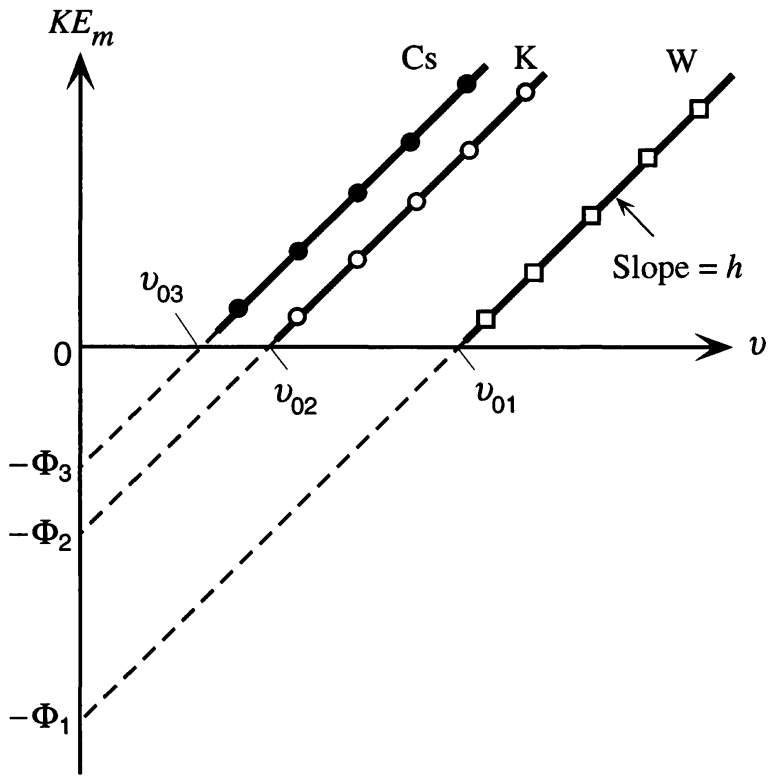


Figure 3.6 The effect of varying the frequency of light and the cathode material in the photoelectric experiment. The lines for the different materials have the same slope h but different intercepts.

Since the magnitude of the saturation photocurrent depends on the light intensity I, whereas the KE of the emitted electron is independent of I, we are forced to conclude that only the *number* of electrons ejected depends on the light intensity. Furthermore, if we plot KE_m (from the V_0 value) against the light frequency ν for different electrode metals for the cathode, we find the typical behavior shown in Figure 3.6. This shows that the KE of the emitted electron depends on the frequency of light. The experimental results shown in Figure 3.6 can be summarized by a statement that relates the KE_m of the electron to the frequency of light and the electrode metal, as follows:

Photoemitted electron maximum KE

$$KE_m = h\nu - h\nu_0 \qquad [3.4]$$

where h is the slope of the straight line and is independent of the type of metal, whereas ν_0 depends on the electrode material for the photocathode (*e.g.*, ν_{01}, ν_{02}, etc.). Equation 3.4 is essentially a succinct statement of the experimental observations of the photoelectric effect as exhibited in Figure 3.6. The constant h is called **Planck's constant,** which, from the slope of the straight lines in Figure 3.6, can be shown to be about 6.6×10^{-34} J s. This was beautifully demonstrated by Millikan in 1915, in an excellent series of photoelectric experiments using different photocathode materials.

The successful interpretation of the photoelectric effect was first given in 1905 by Einstein, who proposed that light consists of "energy packets," each of which has the magnitude $h\nu$. We can call these energy quanta **photons.** When one photon strikes an electron, its energy is transferred to the electron. The whole photon becomes absorbed by the electron. Yet, an electron in a metal is in a lower state of potential energy (PE) than in vacuum, by an amount Φ, which we call the **work function** of the metal, as illustrated in Figure 3.7. The lower PE is what keeps the electron in the metal; otherwise, it would "drop out."

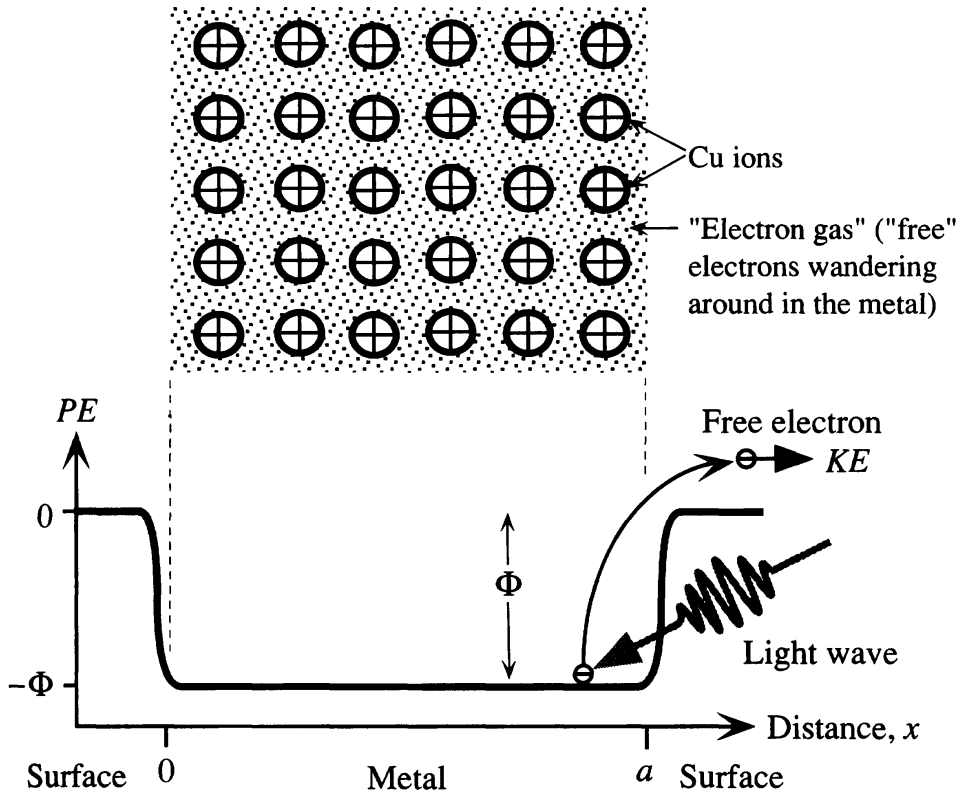


Figure 3.7 The *PE* of an electron inside the metal is lower than outside by an energy called the workfunction of the metal.
Work must be done to remove the electron from the metal.

This lower *PE* is a result of the Coulombic attraction interaction between the electron and the positive metal ions. Some of the photon energy $h\nu$ therefore goes toward overcoming this *PE* barrier. The energy that is left ($h\nu - \Phi$) gives the electron its *KE*. The work function Φ changes from one metal to another. Photoemission only occurs when $h\nu$ is greater than Φ. This is clearly borne out by experiment, since a critical frequency ν_0 is needed to register a photocurrent. When ν is less than ν_0, even if we use an extremely intense light, no current exists because no photoemission occurs, as demonstrated by the experimental results in Figure 3.6. Inasmuch as Φ depends on the metal, so does ν_0. Therefore, in Einstein's interpretation $h\nu_0 = \Phi$. In fact, the measurement of ν_0 constitutes one method of determining the work function of the metal.

This explanation for the photoelectric effect is further supported by the fact that the work function Φ from $h\nu_0$ is in good agreement with that from thermionic emission experiments. There is an apparent similarity between the *I–V* characteristics of the phototube and that of the vacuum tube used in early radios. The only difference is that in the vacuum tube, the emission of electrons from the cathode is achieved by heating the cathode. Thermal energy ejects some electrons over the *PE* barrier Φ. The measurement of Φ by this thermionic emission process agrees with that from photoemission experiments.

In the photonic interpretation of light, we still have to resolve the meaning of the intensity of light, because the classical intensity in Equation 3.2

$$I = \frac{1}{2} c\varepsilon_o \mathcal{E}_o^2 \qquad \textit{Classical light intensity}$$

is obviously not acceptable. Increasing the intensity of illumination in the photoelectric experiment increases the saturation current, which means that more electrons are

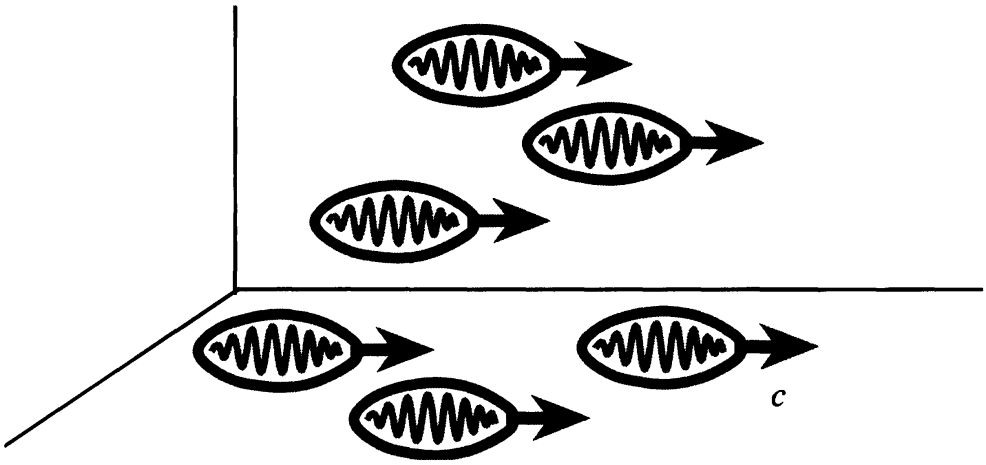


Figure 3.8 Intuitive visualization of light consisting of a stream of photons (not to be taken too literally).
SOURCE: R. Serway, C. J. Moses, and C. A. Moyer, *Modern Physics*, Saunders College Publishing, 1989, p. 56, figure 2.16(b).

emitted per unit time. We therefore infer that the cathode must be receiving more photons per unit time at higher intensities. By definition, "intensity" refers to the amount of energy flowing through a unit area per unit time. If the number of photons crossing a unit area per unit time is the **photon flux,** denoted by Γ_{ph}, then the flow of energy through a unit area per unit time, the **light intensity,** is the product of this photon flux and the energy per photon, that is,

Light intensity

$$I = \Gamma_{ph} h\nu \qquad [3.5]$$

where

Photon flux

$$\Gamma_{ph} = \frac{\Delta N_{ph}}{A \Delta t} \qquad [3.6]$$

in which ΔN_{ph} is the net number of photons crossing an area A in time Δt. With the energy of a photon given as $h\nu$ and the intensity of light defined as $\Gamma_{ph} h\nu$, the explanation for the photoelectric effect becomes self-consistent. The interpretation of light as a stream of photons can perhaps be intuitively imagined as depicted in Figure 3.8.

EXAMPLE 3.1 **ENERGY OF A BLUE PHOTON** What is the energy of a blue photon that has a wavelength of 450 nm?

SOLUTION

The energy of the photon is given by

$$E_{ph} = h\nu = \frac{hc}{\lambda} = \frac{(6.6 \times 10^{-34}\ \text{J s})(3 \times 10^{8}\ \text{m s}^{-1})}{450 \times 10^{-9}\ \text{m}} = 4.4 \times 10^{-19}\ \text{J}$$

Generally, with such small energy values, we prefer electron–volts (eV), so the energy of the photon is

$$\frac{4.4 \times 10^{-19}\ \text{J}}{1.6 \times 10^{-19}\ \text{J/eV}} = 2.75\ \text{eV}$$

EXAMPLE 3.2

THE PHOTOELECTRIC EXPERIMENT In the photoelectric experiment, green light, with a wavelength of 522 nm, is the longest-wavelength radiation that can cause the photoemission of electrons from a clean sodium surface.

a. What is the work function of sodium, in electron–volts?

b. If UV (ultraviolet) radiation of wavelength 250 nm is incident to the sodium surface, what will be the kinetic energy of the photoemitted electrons, in electron–volts?

c. Suppose that the UV light of wavelength 250 nm has an intensity of 20 mW cm^{-2}. If the emitted electrons are collected by applying a positive bias to the opposite electrode, what will be the photoelectric current density?

SOLUTION

a. At threshold, the photon energy just causes photoemissions; that is, the electron just overcomes the potential barrier Φ. Thus, $hc/\lambda_0 = e\Phi$, where Φ is the work function in eV, and λ_0 is the longest wavelength.

$$\Phi = \frac{hc}{e\lambda_0} = \frac{(6.626 \times 10^{-34}\,\text{J s})(3 \times 10^{8}\,\text{m s}^{-1})}{(1.6 \times 10^{-19}\,\text{J/eV})(522 \times 10^{-9}\,\text{m})} = 2.38\ \text{eV}$$

b. The energy of the incoming photon E_{ph} is (hc/λ), so the excess energy over $e\Phi$ goes to the kinetic energy of the electron. Thus,

$$KE = \frac{hc}{e\lambda} - \Phi = \frac{(6.626 \times 10^{-34}\,\text{J s})(3 \times 10^{8}\,\text{m s}^{-1})}{(1.6 \times 10^{-19}\,\text{J/eV})(250 \times 10^{-9}\,\text{m})} - 2.38\ \text{eV} = 2.58\ \text{eV}$$

c. The light intensity (defined as energy flux) is given by $I = \Gamma_{ph}(hc/\lambda)$, where Γ_{ph} is the number of photons arriving per unit area per unit time; that is, photon flux and (hc/λ) is the energy per photon. Thus, if each photon releases one electron, the electron flux will be equal to the photon flux, and the current density, which is the charge flux, will be

$$J = e\Gamma_{ph} = \frac{eI\lambda}{hc} = \frac{(1.6 \times 10^{-19}\,\text{C})(20 \times 10^{-3} \times 10^{4}\,\text{J s}^{-1}\,\text{m}^{-2})(250 \times 10^{-9}\,\text{m})}{(6.626 \times 10^{-34}\,\text{J s})(3 \times 10^{8}\,\text{m s}^{-1})}$$

$$= 40.3\ \text{A m}^{-2} \quad \text{or} \quad 4.0\ \text{mA cm}^{-2}$$

3.1.3 COMPTON SCATTERING

When an X-ray strikes an electron, it is deflected, or "scattered." In addition, the electron moves away after the interaction, as depicted in Figure 3.9. The wavelength of the incoming and scattered X-rays can readily be measured. The frequency ν' of the scattered X-ray is less than the frequency ν of the incoming X-ray. When the *KE* of the electron is determined, we find that

$$KE = h\nu - h\nu'$$

Since the electron now also has a momentum p_e, then from the conservation of linear momentum law, we are forced to accept that the X-ray also has a momentum. The Compton effect experiments showed that the momentum of the photon is related to its wavelength by

$$p = \frac{h}{\lambda} \qquad [3.7]$$

Momentum of a photon

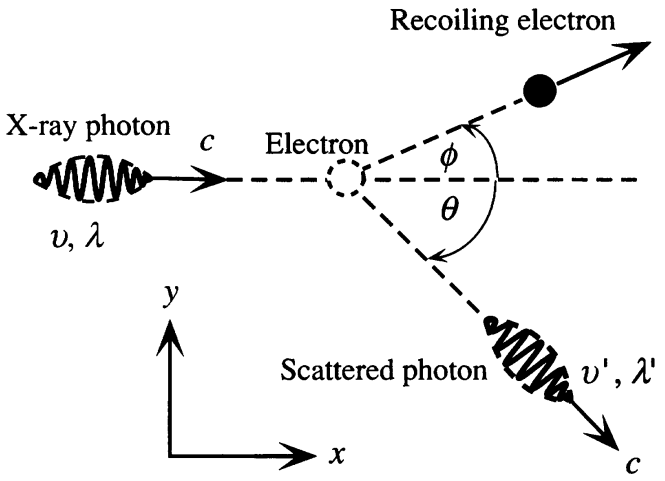


Figure 3.9 Scattering of an X-ray photon by a "free" electron in a conductor.

We see that a photon not only has an energy $h\nu$, but also a momentum p, and it interacts as if it were a discrete entity like a particle. Therefore, when discussing the properties of a photon, we must consider its energy and momentum as if it were a particle.

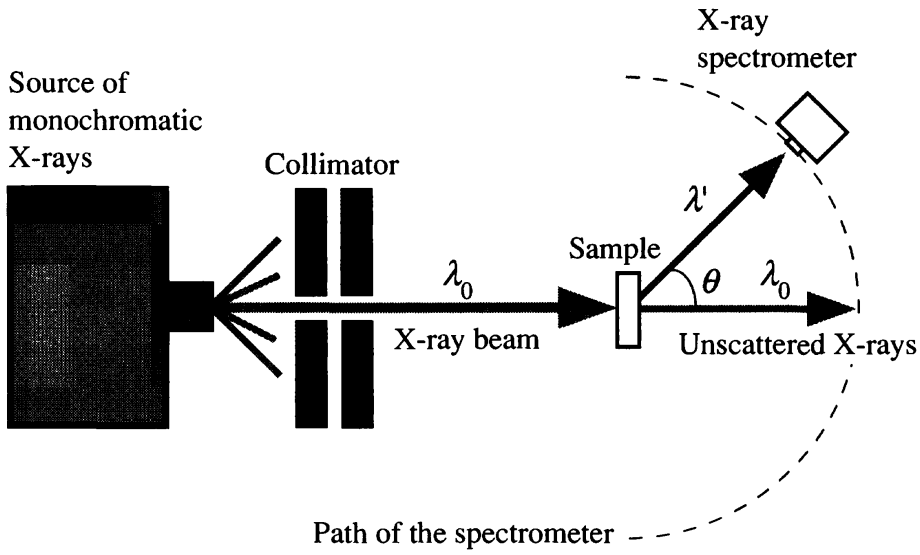
We should mention that the description of the Compton effect shown in Figure 3.9 is, in fact, the inference from a more practical experiment involving the scattering of X-rays from a metal target. A collimated monochromatic beam of X-rays of wavelength λ_0 strikes a conducting target, such as graphite, as illustrated in Figure 3.10a. A conducting target contains a large number of nearly "free" electrons (conduction electrons), which can scatter the X-rays. The scattered X-rays are detected at various angles θ with respect to the original direction, and their wavelength λ' is measured. The result of the experiment is therefore the scattered wavelength λ' measured at various scattering angles θ, as shown in Figure 3.10b. It turns out that the λ' versus θ results agree with the conservation of linear momentum law applied to an X-ray photon colliding with an electron with the momentum of the photon given precisely by Equation 3.7.

The photoelectric experiment and the Compton effect are just two convincing experiments in modern physics that force us to accept that light can have particle-like properties. We already know that it can also exhibit wave-like properties, in such experiments as Young's interference fringes. We are then faced with what is known as the wave–particle dilemma. How do we know whether light is going to behave like a wave or a particle? The properties exhibited by light depend very much on the nature of the experiment. Some experiments will require the wave model, whereas others may use the particulate interpretation of light. We should perhaps view the two interpretations as two complementary ways of modeling the behavior of light when it interacts with matter, accepting the fact that light has a dual nature. Both models are needed for a full description of the behavior of light.

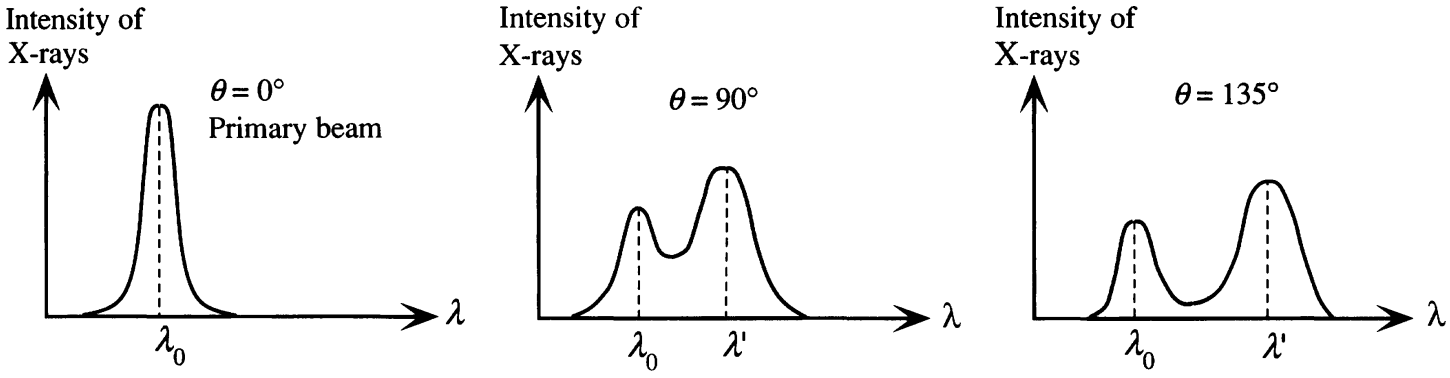
Photon energy and momentum

The expressions for the energy and momentum of the photon, $E = h\nu$ and $p = h/\lambda$, can also be written in terms of the angular frequency $\omega(= 2\pi\nu)$ and the wave number k, defined as $k = 2\pi/\lambda$. If we define $\hbar = h/2\pi$, then

$$E = h\nu = \hbar\omega \qquad \text{and} \qquad p = \frac{h}{\lambda} = \hbar k \qquad \textbf{[3.8]}$$



(a) A schematic diagram of the Compton experiment



(b) Results from the Compton experiment

Figure 3.10 The Compton experiment and its results.

EXAMPLE 3.3

X-RAY PHOTON ENERGY AND MOMENTUM X-rays are photons with very short wavelengths that can penetrate or pass through objects, hence their use in medical imaging, security scans at airports, and many other applications including X-ray diffraction studies of crystal structures. Typical X-rays used in mammography (medical imaging of breasts) have a wavelength of about 0.6 angstrom (1 Å = 10^{-10} m). Calculate the energy and momentum of an X-ray photon with this wavelength, and the velocity of a *corresponding* electron that has the same momentum.

SOLUTION

The photon energy E_{ph} is given by

$$E_{ph} = h\nu = \frac{hc}{\lambda} = \frac{(6.6 \times 10^{-34}\ \text{J s})(3 \times 10^{8}\ \text{m s}^{-1})}{0.6 \times 10^{-10}\ \text{m}} \times \frac{\text{eV J}^{-1}}{1.6 \times 10^{-19}}$$

$$= 2.06 \times 10^{4}\ \text{eV} \quad \text{or} \quad 20.6\ \text{keV}$$

The momentum p of this X-ray photon is

$$p = \frac{h}{\lambda} = \frac{6.6 \times 10^{-34}\ \text{J s}}{0.6 \times 10^{-10}\ \text{m}} = 1.1 \times 10^{-23}\ \text{kg m s}^{-1}$$

A corresponding electron with the same momentum, $m_e v_{\text{electron}} = p$, would have a velocity

$$v_{\text{electron}} = \frac{p}{m_e} = \frac{1.1 \times 10^{-23}\ \text{kg m s}^{-1}}{9.1 \times 10^{-31}\ \text{kg}} = 1.2 \times 10^{7}\ \text{m s}^{-1}$$

This is much greater than the average speed of conduction (free) electrons whizzing around inside a metal, which is $\sim 10^6$ m s^{-1}.

3.1.4 BLACK BODY RADIATION

Experiments indicate that all objects emit and absorb energy in the form of radiation, and the intensity of this radiation depends on the radiation wavelength and temperature of the object. This radiation is frequently termed **thermal radiation.** When the object is in thermal equilibrium with its surroundings, that is, at the same temperature, the object absorbs as much radiation energy as it emits. On the other hand, when the temperature of the object is above the temperature of its surroundings, there is a net emission of radiation energy. The maximum amount of radiation energy that can be emitted by an object is called the **black body radiation.** Although, in general, the intensity of the radiated energy depends on the material's surface, the radiation emitted from a cavity with a small aperture is independent of the material of the cavity and corresponds very closely to black body radiation.

The intensity of the emitted radiation has the spectrum (*i.e.*, intensity vs. wavelength characteristic), and the temperature dependence illustrated in Figure 3.11. It is useful to define a **spectral irradiance** I_λ as the emitted radiation intensity (power per unit area) per unit wavelength, so that $I_\lambda\, \delta\lambda$ is the intensity in a small range of wavelengths $\delta\lambda$. Figure 3.11 shows the typical I_λ versus λ behavior of black body radiation at two temperatures. We assume that the characteristics of the radiation emerging from the aperture represent those of the radiation within the cavity.

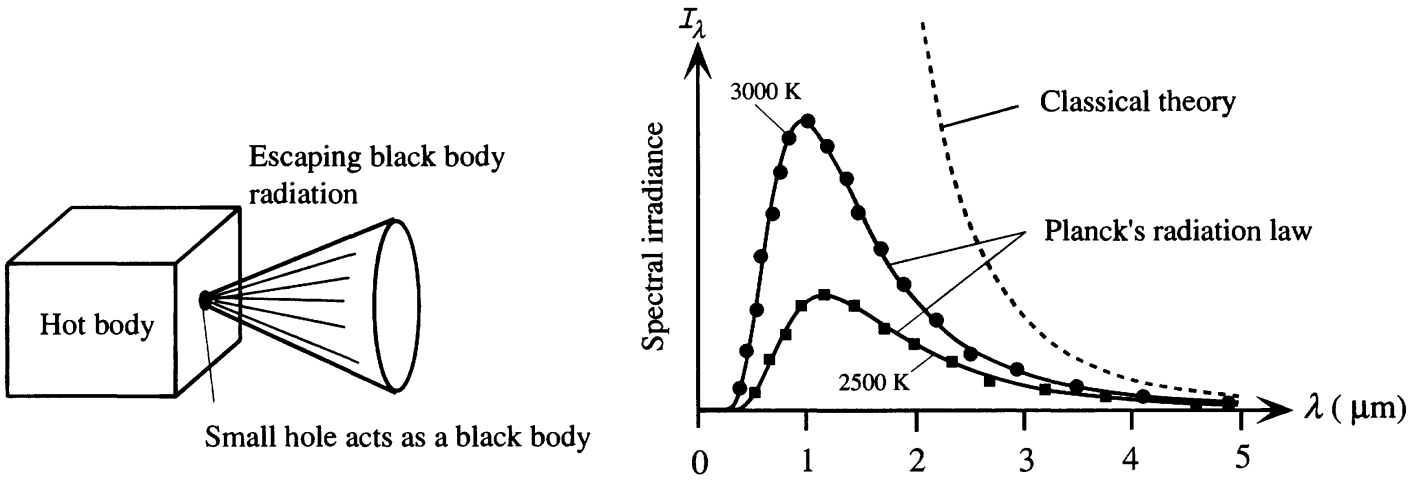


Figure 3.11 Schematic illustration of black body radiation and its characteristics.
Spectral irradiance versus wavelength at two temperatures (3000 K is about the temperature of the incandescent tungsten filament in a light bulb).

Classical physics predicts that the acceleration and deceleration of the charges due to various thermal vibrations, oscillations, or motions of the atoms in the surface region of the cavity material result in electromagnetic waves of the emissions. These waves then interfere with each other, giving rise to many types of standing electromagnetic waves with different wavelengths in the cavity. Each wave contributes an energy kT to the emitted intensity. If we calculate the number of standing waves within a small range of wavelength, the classical prediction leads to the **Rayleigh–Jeans law** in which $I_\lambda \propto 1/\lambda^4$ and $I_\lambda \propto T$, which are not in agreement with the experiment, especially in the short-wavelength range (see Figure 3.11).

Max Planck (1900) was able to show that the experimental results can be explained if we assume that the radiation within the cavity involves the emission and absorption of discrete amounts of light energy by the oscillation of the molecules of the cavity material. He assumed that oscillating molecules emit and absorb a quantity of energy that is an integer multiple of a discrete energy quantum that is determined by the frequency ν of the radiation and given by $h\nu$. This is what we now call a photon. He then considered the energy distribution (the statistics) in the molecular oscillations and took the probability of an oscillator possessing an energy $nh\nu$ (where n is an integer) to be proportional to the Boltzmann factor, $\exp(-nh\nu/kT)$. He eventually derived the mathematical form of the black body radiation characteristics in Figure 3.11. Planck's black body radiation formula for I_λ is generally expressed as

$$I_\lambda = \frac{2\pi hc^2}{\lambda^5\left[\exp\left(\frac{hc}{\lambda kT}\right) - 1\right]} \qquad [3.9]$$

Planck's radiation law

where k is the Boltzmann constant. Planck's radiation law based on the emission and absorption of photons is in excellent agreement with all observed black body radiation characteristics as depicted in Figure 3.11.

Planck's radiation law is undoubtedly one of the major successes of modern physics. We can take Equation 3.9 one step further and derive *Stefan's black body radiation law* that was used in Chapter 2 to calculate the rate of radiation energy emitted from the hot filament of a light bulb. If we integrate I_λ over all wavelengths,[2] we will obtain the total radiative power P_S emitted by a black body per unit surface area at a temperature T,

$$P_S = \int_0^\infty I_\lambda \, d\lambda = \left(\frac{2\pi^5 k^4}{15c^2h^3}\right)T^4 = \sigma_S T^4 \qquad [3.10]$$

Stefan's black body radiation law

where

$$\sigma_S = \frac{2\pi^5 k^4}{15c^2h^3} = 5.670 \times 10^{-8}\ \mathrm{W\ m^{-2}\ K^{-4}} \qquad [3.11]$$

Stefan's constant

[2] The integration of Equation 3.9 can be done by looking up definite integral tables in math handbooks—we only need the result of the mathematics, which is Equation 3.10. The P_S in Equation 3.10 is sometimes called the *radiant emittance*. Stefan's law is also known as the Stefan-Boltzmann law.

Equation 3.10 in which $P_S = \sigma_S T^4$ is **Stefan's law** for black body radiation, and the σ_S in Equation 3.11 is the **Stefan constant** with a value of approximately 5.67×10^{-8} W m^{-2} K^{-4}. Stefan's law was known before Planck used quantum physics to derive his black body radiation law embedded in I_λ. A complete explanation of Stefan's law and the value for σ_S however had to wait for Planck's law. The h in Equation 3.10 or 3.11 is a clear pointer that the origin of Stefan's law lies in quantum physics.

EXAMPLE 3.4 **STEFAN'S LAW AND THE LIGHT BULB** Stefan's law as stated in Equation 3.10 applies to a perfect black body that is emitting radiation into its environment which is at absolute zero. If the environment or the surroundings of the black body is at a finite temperature T_o, than the surroundings would also be emitting radiation. The same black body will then also absorb radiation from its environment. By definition, a black body is not only a perfect emitter of radiation but also a perfect absorber of radiation. The rate of radiation absorbed from the environment per unit surface is again given by Equation 3.10 but with T_o instead of T since it is the surroundings that are emitting the radiation. Thus, $\sigma_S T_o^4$ is the absorbed radiation rate from the surroundings, so

$$\text{Net rate of radiative power emission per unit surface} = \sigma_S T^4 - \sigma_S T_o^4$$

Further, not all surfaces are perfect black bodies. Black body emission is the maximum possible emission from a surface at a given temperature. A real surface emits less than a black body. **Emissivity** ε of a surface measures the efficiency of a surface in terms of a black body emitter; it is the ratio of the emitted radiation from a real surface to that emitted from a black body at a given temperature and over the same wavelength range. The *total* net rate of radiative power emission becomes

Stefan's law for a real surface

$$P_{\text{radiation}} = S\varepsilon\sigma_S(T^4 - T_o^4) \qquad \textbf{[3.12]}$$

where S is the surface area that is emitting the radiation. Consider the tungsten filament of a 100 W light bulb in a lamp. When we switch the lamp on, the current through the filament generates heat which quickly heats up the filament to an operating temperature T_f. At this temperature, the electric energy that is input into the bulb is radiated away from the filament as radiation energy. A typical 100 W bulb filament has a length of 57.9 cm and a diameter of 63.5 μm. Its surface area is then

$$S = \pi(63.5 \times 10^{-6}\text{ m})(0.579\text{ m}) = 1.155 \times 10^{-4}\text{ m}^2$$

The emissivity ε of tungsten is about 0.35. Assuming that under steady-state operation all the electric power that is input into the bulb's filament is radiated away,

$$\begin{aligned} 100\text{ W} = P_{\text{radiation}} &= S\varepsilon\sigma_S(T_f^4 - T_o^4) \\ &= (1.155 \times 10^{-4}\text{ m}^2)(0.35)(5.67 \times 10^{-8}\text{ W m}^{-2}\text{ K}^{-4})(T_f^4 - 300^4) \end{aligned}$$

Solving we find,

$$T_f = 2570\text{ K} \qquad \text{or} \qquad 2297\text{ °C}$$

which is well below the melting temperature of tungsten which is 3422 °C. The second term that has T_o^4 has very little effect on the calculation as radiation absorption from the environment is practically nil compared with the emitted radiation at T_f.

The shift in the spectral intensity emitted from a black body with temperature is of particular interest to many photoinstrumention engineers. The peak spectral intensity in Figure 3.11 occurs at a wavelength λ_{max}, which, by virtue of Equation 3.9, depends on the temperature of

the black body. By substituting a new variable $x = hc/(kT\lambda)$ into Equation 3.9 and differentiating it, or plotting it against x, we can show that the peak occurs when

$$\lambda_{max} T \approx 2.89 \times 10^{-3} \text{ m K}$$

Wien's displacement law

which is known as **Wien's displacement law.** The peak emission shifts to lower wavelengths as the temperature increases. We can calculate the wavelength λ_{max} corresponding to the peak in the spectral distribution of emitted radiation from our 100 W lamp: $\lambda_{max} = (2.89 \times 10^{-3} \text{ m K})/(2570 \text{ K}) = 1.13 \text{ μm}$ (in the infrared).

3.2 THE ELECTRON AS A WAVE

3.2.1 DE BROGLIE RELATIONSHIP

It is apparent from the photoelectric and Compton effects that light, which we thought was a wave, can behave as if it were a stream of particulate-like entities called photons. Can electrons exhibit wave-like properties? Again, this depends on the experiment and on the energy of the electrons.

When the interference and diffraction experiments in Figures 3.2 and 3.3 are repeated with an electron beam, very similar results are found to those obtainable with light and X-rays. When we use an electron beam in Young's double-slit experiment, we observe high- and low-intensity regions (*i.e.*, Young's fringes), as illustrated in Figure 3.12. The interference pattern is viewed on a fluorescent TV screen. When an energetic electron beam hits an Al polycrystalline sample, it produces diffraction rings on a fluorescent screen (Figure 3.13), just like X-rays do on a photographic

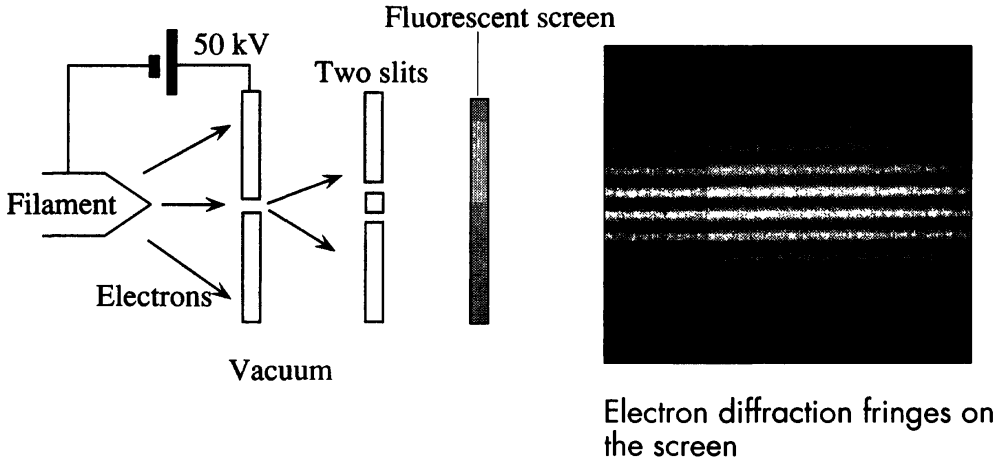
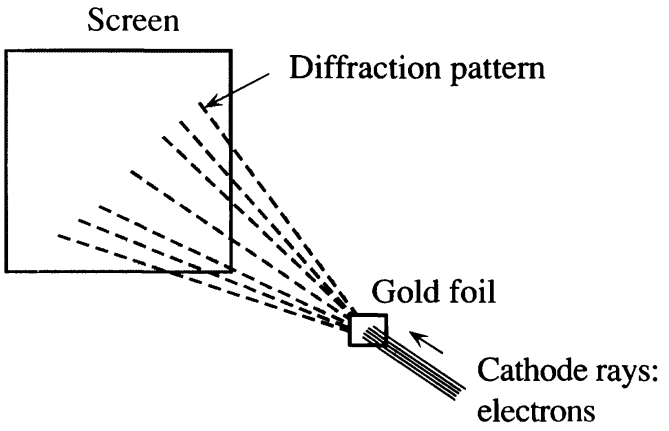


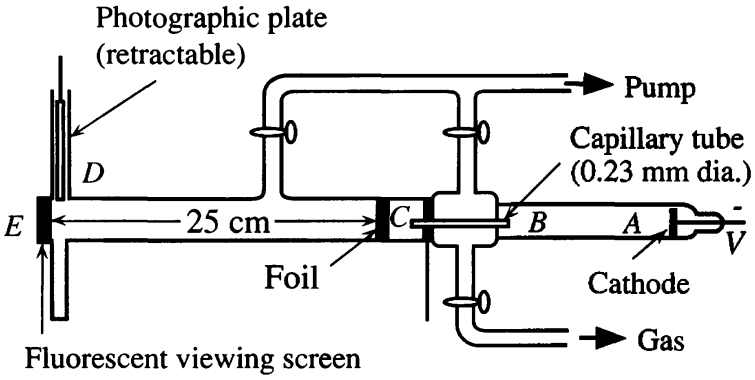
Figure 3.12 Young's double-slit experiment with electrons involves an electron gun and two slits in a cathode ray tube (CRT) (hence, in vacuum).

Electrons from the filament are accelerated by a 50 kV anode voltage to produce a beam that is made to pass through the slits. The electrons then produce a visible pattern when they strike a fluorescent screen (*e.g.*, a TV screen), and the resulting visual pattern is photographed.

SOURCE: Pattern from C. Jönsson, D. Brandt, and S. Hirschi, *Am. J. Physics*, **42**, 1974, p. 9, figure 8. Used with permission.

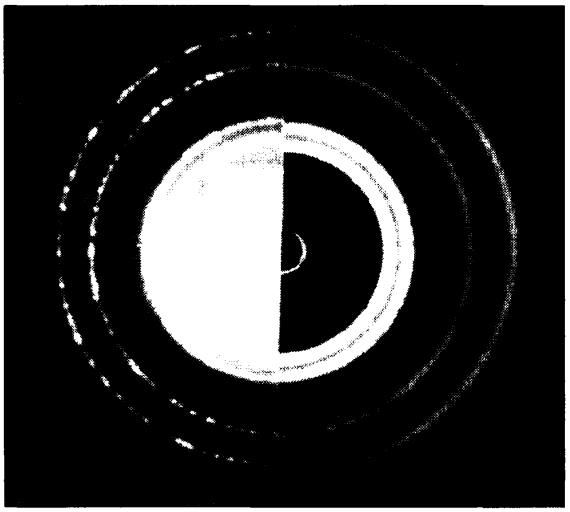


(a) Thomson diffracted electrons by using a thin gold foil and produced a diffraction pattern on the screen of his apparatus in (b). The foil was polycrystalline, so the diffraction pattern was circular rings.

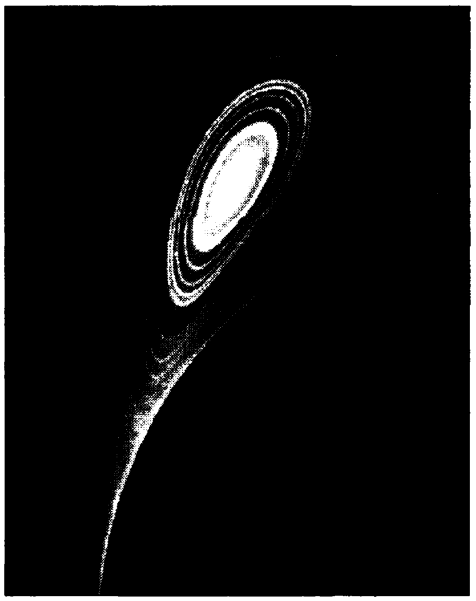


(b) In Thomson's electron diffraction apparatus a beam of electrons is generated in tube *A*, passed through collimating tube *B*, and made to impinge on a thin gold foil *C*. The transmitted electrons impinge on the fluorescent screen *E*, or a photographic plate *D*, which could be lowered into the path. The entire apparatus was evacuated during the experiment.

(c) Electron diffraction pattern obtained by G. P. Thomson using a gold foil target.



(d) Composite photograph showing diffraction patterns produced with an aluminum foil by X-rays and electrons of similar wavelength. Left: X-rays of $\lambda = 0.071$ nm. Right: Electrons of energy 600 eV.



(e) Diffraction pattern produced by 40 keV electrons passing through zinc oxide powder. The distortion of the pattern was produced by a small magnet placed between the sample and the photographic plate. An X-ray diffraction pattern would not be affected by a magnetic field.

Figure 3.13 The diffraction of electrons by crystals gives typical diffraction patterns that would be expected if waves were being diffracted, as in X-ray diffraction with crystals.

SOURCE: (b) from G. P. Thomson, *Proceedings of the Royal Society*, A117, no. 600, 1928; (c) and (d) from A. P. French and F. Taylor, *An Introduction to Quantum Mechanics*, Norton, New York, 1978, p. 75; (e) from R. B. Leighton, *Principles of Modern Physics*, New York: McGraw-Hill, 1959, p. 84.

plate. The diffraction pattern obtained with an electron beam (Figure 3.13) means that the electrons are obeying the Bragg diffraction condition $2d \sin\theta = n\lambda$ just as much as the X-ray waves.

Since we know the interatomic spacing d and we can measure the angle of diffraction 2θ, we can readily evaluate the wavelength λ associated with the wave-like behavior of the electrons. Furthermore, from the accelerating voltage V in the electron tube, we can also determine the momentum of the electrons, because the kinetic energy gained by the electrons, $(p^2/2m_e)$, is equal to eV. Simply by adjusting the accelerating voltage V, we can therefore study how the wavelength of the electron depends on the momentum.

As a result of such studies and other similar experiments, it has been found that an electron traveling with a momentum p behaves like a wave of wavelength λ given by

$$\lambda = \frac{h}{p} \qquad [3.13]$$

Wavelength of the electron

This is just the reverse of the equation for the momentum of a photon given its wavelength. The same equation therefore relates wave-like and particle-like properties to and from each other. Thus,

$$\lambda = \frac{h}{p} \quad \text{or} \quad p = \frac{h}{\lambda}$$

De Broglie relations

is an equation that exposes the wave–particle duality of nature. It was first hypothesized by De Broglie in 1924. As an example, we can calculate the wavelengths of a number of particle-like objects:

a. A 50 gram golf ball traveling at a velocity of 20 m s^{-1}.

The wavelength is

$$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}\,\text{J s}}{(50 \times 10^{-3}\,\text{kg})(20\,\text{m s}^{-1})} = 6.63 \times 10^{-34}\,\text{m}$$

The wavelength is so small that this golf ball will not exhibit any wave effects. Firing a stream of golf balls at a wall will not result in "diffraction rings" of golf balls.

b. A proton traveling at 2200 m s^{-1}.

Using $m_p = 1.67 \times 10^{-27}$ kg, we have $\lambda = (h/mv) \approx 0.18$ nm. This is only slightly smaller than the interatomic distance in crystals, so firing protons at a crystal can result in diffraction. (Recall that to get a diffraction peak, we must satisfy the Bragg condition, $2d \sin\theta = n\lambda$.) Protons, however, are charged, so they can penetrate only a small distance into the crystal. Hence, they are not used in crystal diffraction studies.

c. Electron accelerated by 100 V.

This voltage accelerates the electron to a KE equal to eV. From $KE = p^2/2m_e = eV$, we can calculate p and hence $\lambda = h/p$. The result is $\lambda = 0.123$ nm. Since this is comparable to typical interatomic distances in solids, we would see a diffraction pattern when an electron beam strikes a crystal. The actual pattern is determined by the Bragg diffraction condition.

3.2.2 TIME-INDEPENDENT SCHRÖDINGER EQUATION

The experiments in which electrons exhibit interference and diffraction phenomena show quite clearly that, under certain conditions, the electron can behave as a wave; in other words, it can exhibit wave-like properties. There is a general equation that describes this wave-like behavior and, with the appropriate potential energy and boundary conditions, will predict the results of the experiments. The equation is called the **Schrödinger equation** and it forms the foundations of quantum theory. Its fundamental nature is analogous to the classical physics assertion of Newton's second law, $F = ma$, which of course cannot be proved. As a fundamental equation, Schrödinger's has been found to successfully predict every observable physical phenomenon at the atomic scale. Without this equation, we will not be able to understand the properties of electronic materials and the principles of operation of many semiconductor devices. We introduce the equation through an analogy.

A traveling electromagnetic wave resulting from sinusoidal current oscillations, or the traveling voltage wave on a long transmission line, can generally be described by a traveling-wave equation of the form

$$\mathcal{E}(x, t) = \mathcal{E}_o \exp j(kx - \omega t) = \mathcal{E}(x) \exp(-j\omega t) \qquad [3.14]$$

where $\mathcal{E}(x) = \mathcal{E}_0 \exp(jkx)$ represents the spatial dependence, which is separate from the time variation. We assume that no transients exist to upset this perfect sinusoidal propagation. We note that the time dependence is harmonic and therefore predictable. For this reason, in ac circuits we put aside the $\exp(-j\omega t)$ term until we need the instantaneous magnitude of the voltage.

The average intensity $I_{\text{av}} = \frac{1}{2} c\varepsilon_o \mathcal{E}_o^2$ depends on the square of the amplitude. In Young's double-slit experiment, the intensity varies along the y direction, which means that $\mathcal{E}_o^2$ for the resultant wave depends on y. In the electron version of this experiment in Figure 3.12, what changes in the y direction is the probability of observing electrons; that is, there are peaks and troughs in the probability of finding electrons along y, just like the $\mathcal{E}_o^2$ variation along y. We should therefore attach some probability interpretation to the wave description of the electron.

In 1926, Max Born suggested a probability wave interpretation for the wave-like behavior of the electron.

$$\mathcal{E}(x, t) = \mathcal{E}_o \sin(kx - \omega t)$$

is a plane traveling **wavefunction** for an electric field; experimentally, we measure and interpret the *intensity* of a wave, namely $|\mathcal{E}(x, t)|^2$. There may be a similar wave function for the electron, which we can represent by a function $\Psi(x, t)$. According to Born, the significance of $\Psi(x, t)$ is that its amplitude squared represents the probability of finding the electron per unit distance. Thus, in three dimensions, if $\Psi(x, y, z, t)$ represents the wave property of the electron, it must have one of the following interpretations:

$|\Psi(x, y, z, t)|^2$ is the probability of finding the electron per unit volume at x, y, z at time t.

$|\Psi(x, y, z, t)|^2 \, dx \, dy \, dz$ is the probability of finding the electron in a small elemental volume $dx \, dy \, dz$ at x, y, z at time t.

If we are just considering one dimension, then the wavefunction is $\Psi(x, t)$, and $|\Psi(x, t)|^2\, dx$ is the probability of finding the electron between x and $(x + dx)$ at time t.

We should note that since only $|\Psi|^2$ has meaning, not Ψ, the latter function need not be real; it can be a complex function with real and imaginary parts. For this reason, we tend to use $\Psi^*\,\Psi$, where Ψ^* is the complex conjugate of Ψ, instead of $|\Psi|^2$, to represent the probability per unit volume.

To obtain the wavefunction $\Psi(x, t)$ for the electron, we need to know how the electron interacts with its environment. This is embodied in its potential energy function $V = V(x, t)$, because the net force the electron experiences is given by

$$F = -dV/dx.$$

For example, if the electron is attracted by a positive charge (*e.g.*, the proton in a hydrogen atom), then it clearly has an electrostatic potential energy given by

$$V(r) = -\frac{e^2}{4\pi\varepsilon_o r}$$

where $r = \sqrt{x^2 + y^2 + z^2}$ is the distance between the electron and the proton.

If the *PE* of the electron is time independent, which means that $V = V(x)$ in one dimension, then the spatial and time dependences of $\Psi(x, t)$ can be separated, just as in Equation 3.14, and the **total wavefunction** $\Psi(x, t)$ of the electron can be written as

Steady-state total wave function

$$\Psi(x, t) = \psi(x) \exp\left(-\frac{jEt}{\hbar}\right) \qquad [3.15]$$

where $\psi(x)$ is the electron wavefunction that describes only the spatial behavior, and E is the energy of the electron. The temporal behavior is simply harmonic, by virtue of $\exp(-jEt/\hbar)$, which corresponds to $\exp(-j\omega t)$ with an angular frequency $\omega = E/\hbar$. The fundamental equation that describes the electron's behavior by determining $\psi(x)$ is called the **time-independent Schrödinger equation.** It is given by the famous equation

Schrödinger's equation for one dimension

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \qquad [3.16a]$$

where m is the mass of the electron.

This is a second-order differential equation. It should be reemphasized that the potential energy V in Equation 3.16a depends only on x. If the potential energy of the electron depends on time as well, that is, if $V = V(x, t)$, then in general $\Psi(x, t)$ cannot be written as $\psi(x)\exp(-jEt/\hbar)$. Instead, we must use the full version of the Schrödinger equation, which is discussed in more advanced textbooks.

In three dimensions, there will be derivatives of ψ with respect to x, y, and z. We use the calculus notation $(\partial\psi/\partial x)$, differentiating $\psi(x, y, z)$ with respect to x but keeping y and z constant. Similar notations $\partial\psi/\partial y$ and $\partial\psi/\partial z$ are used for derivatives with respect to y alone and with respect to z alone, respectively. In three dimensions, Equation 3.16a becomes

Schrödinger's equation for three dimensions

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \qquad [3.16b]$$

where $V = V(x, y, z)$ and $\psi = \psi(x, y, z)$.

Equation 3.16b is a fundamental equation, called the time-independent Schrödinger equation, the solution of which gives the steady-state behavior of the electron in a time-independent potential energy environment described by $V = V(x, y, z)$. By solving Equation 3.16b, we will know the probability distribution and the energy of the electron. Once $\psi(x, y, z)$ has been determined, the total wavefunction for the electron is given by Equation 3.15 so that

$$|\Psi(x, y, z, t)|^2 = |\psi(x, y, z)|^2$$

which means that the steady-state probability distribution of the electron is simply $|\psi(x, y, z)|^2$.

The time-independent Schrödinger equation can be viewed as a "mathematical crank." We input the potential energy of the electron and the boundary conditions, turn the crank, and get the probability distribution and the energy of the electron under steady-state conditions.

Two important boundary conditions are often used to solve the Schrödinger equation. First, as an analogy, when we stretch a string between two fixed points and put it into a steady-state vibration, there are no discontinuities or kinks along the string. We can therefore intelligently guess that because $\psi(x)$ represents wave-like behavior, it must be a smooth function without any discontinuities.

The first boundary condition is that Ψ must be continuous, and the second is that $d\Psi/dx$ must be continuous. In the steady state, these two conditions translate directly to ψ and $d\psi/dx$ being continuous. Since the probability of finding the electron is represented by $|\psi|^2$, this function must be single-valued and smooth, without any discontinuities, as illustrated in Figure 3.14. The enforcement of these boundary conditions results in strict requirements on the wavefunction $\psi(x)$, as a result of which only certain wavefunctions are acceptable. These wavefunctions are called the **eigenfunctions** (characteristic functions) of the system, and they determine the behavior and energy of the electron under steady-state conditions. The eigenfunctions $\psi(x)$ are also called **stationary states,** inasmuch as we are only considering steady-state behavior.

It is important to note that the Schrödinger equation is generally applicable to all matter, not just the electron. For example, the equation can also be used to describe the behavior of a proton, if the appropriate potential energy $V(x, y, z)$ and mass (m_{proton}) are used. Wavefunctions associated with particles are frequently called **matter waves.**

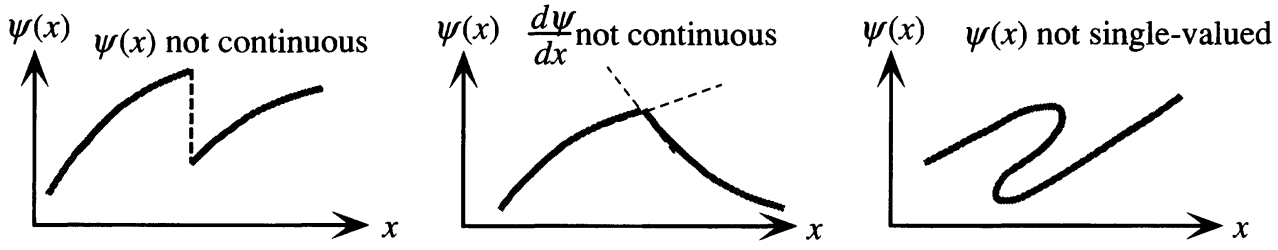


Figure 3.14 Unacceptable forms of $\psi(x)$.

EXAMPLE 3.5

THE FREE ELECTRON Solve the Schrödinger equation for a free electron whose energy is E. What is the uncertainty in the position of the electron and the uncertainty in the momentum of the electron?

SOLUTION

Since the electron is free, its potential energy is zero, $V = 0$. In the Schrödinger equation, this leads to

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

We can write this as

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

where we defined $k^2 = (2m/\hbar^2)E$. Solving the differential equation, we get

$$\psi(x) = A\exp(jkx) \qquad \text{or} \qquad B\exp(-jkx)$$

The total wavefunction is obtained by multiplying $\psi(x)$ by $\exp(-jEt/\hbar)$. We can define a fictitious frequency for the electron by $\omega = E/\hbar$ and multiply $\psi(x)$ by $\exp(-j\omega t)$:

$$\Psi(x,t) = A\exp j(kx - \omega t) \qquad \text{or} \qquad B\exp j(-kx - \omega t)$$

Each of these is a traveling wave. The first solution is a traveling wave in the $+x$ direction, and the second one is in the $-x$ direction. Thus, the free electron has a traveling wave solution with a wavenumber $k = 2\pi/\lambda$, that can have any value. The energy E of the electron is simply KE, so

$$KE = E = \frac{(\hbar k)^2}{2m}$$

When we compare this with the classical physics expression $KE = (p^2/2m)$, we see that the momentum is given by

$$p = \hbar k \qquad \text{or} \qquad p = \frac{h}{\lambda}$$

This is the de Broglie relationship. The latter therefore results naturally from the Schrödinger equation for a free electron.

The probability distribution for the electron is

$$|\psi(x)|^2 = |A\exp j(kx)|^2 = A^2$$

which is constant over the entire space. Thus, the electron can be anywhere between $x = -\infty$ and $x = +\infty$. The uncertainty Δx in its position is infinite. Since the electron has a well-defined wavenumber k, its momentum p is also well-defined by virtue of $p = \hbar k$. The uncertainty Δp in its momentum is thus zero.

EXAMPLE 3.6

WAVELENGTH OF AN ELECTRON BEAM Electrons are accelerated through a 100 V potential difference to strike a polycrystalline aluminum sample. The diffraction pattern obtained indicates that the highest intensity and smallest angle diffraction, corresponding to diffraction from the (111) planes, has a diffraction angle of 30.4°. From X-ray studies, the separation of the (111)

planes is 0.234 nm. What is the wavelength of the electron and how does it compare with that from the de Broglie relationship?

SOLUTION

Since we know the angle of diffraction $2\theta (= 30.4°)$ and the interplanar separation $d (= 0.234$ nm), we can readily calculate the wavelength of the electron from the Bragg condition for diffraction, $2d \sin\theta = n\lambda$. With $n = 1$,

$$\lambda = 2d \sin\theta = 2(0.234 \text{ nm}) \sin(15.2°) = 0.1227 \text{ nm}$$

This is the wavelength of the electron.

When an electron is accelerated through a voltage V, it gains KE equal to eV, so $p^2/2m = eV$ and $p = (2meV)^{1/2}$. This is the momentum imparted by the potential difference V. From the de Broglie relationship, the wavelength should be

$$\lambda = \frac{h}{p} = \frac{h}{(2meV)^{1/2}}$$

or

$$\lambda = \left(\frac{h^2}{2meV}\right)^{1/2}$$

Substituting for e, h, and m, we obtain

$$\lambda = \frac{1.226 \text{ nm}}{V^{1/2}}$$

The experiment uses 100 V, so the de Broglie wavelength is

$$\lambda = \frac{1.226 \text{ nm}}{V^{1/2}} = \frac{1.226 \text{ nm}}{100^{1/2}} = 0.1226 \text{ nm}$$

which is in excellent agreement with that determined from the Bragg condition.

3.3 INFINITE POTENTIAL WELL: A CONFINED ELECTRON

Consider the behavior of the electron when it is confined to a certain region, $0 < x < a$. Its PE is zero inside that region and infinite outside, as shown in Figure 3.15. The electron cannot escape, because it would need an infinite PE. Clearly the probability $|\psi|^2$ of finding the electron per unit volume is zero outside $0 < x < a$. Thus, $\psi = 0$ when $x \leq 0$ and $x \geq a$, and ψ is determined by the Schrödinger equation in $0 < x < a$ with $V = 0$. Therefore, in the region $0 < x < a$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0 \qquad [3.17]$$

This is a second-order linear differential equation. As a general solution, we can take

$$\psi(x) = A \exp(jkx) + B \exp(-jkx)$$

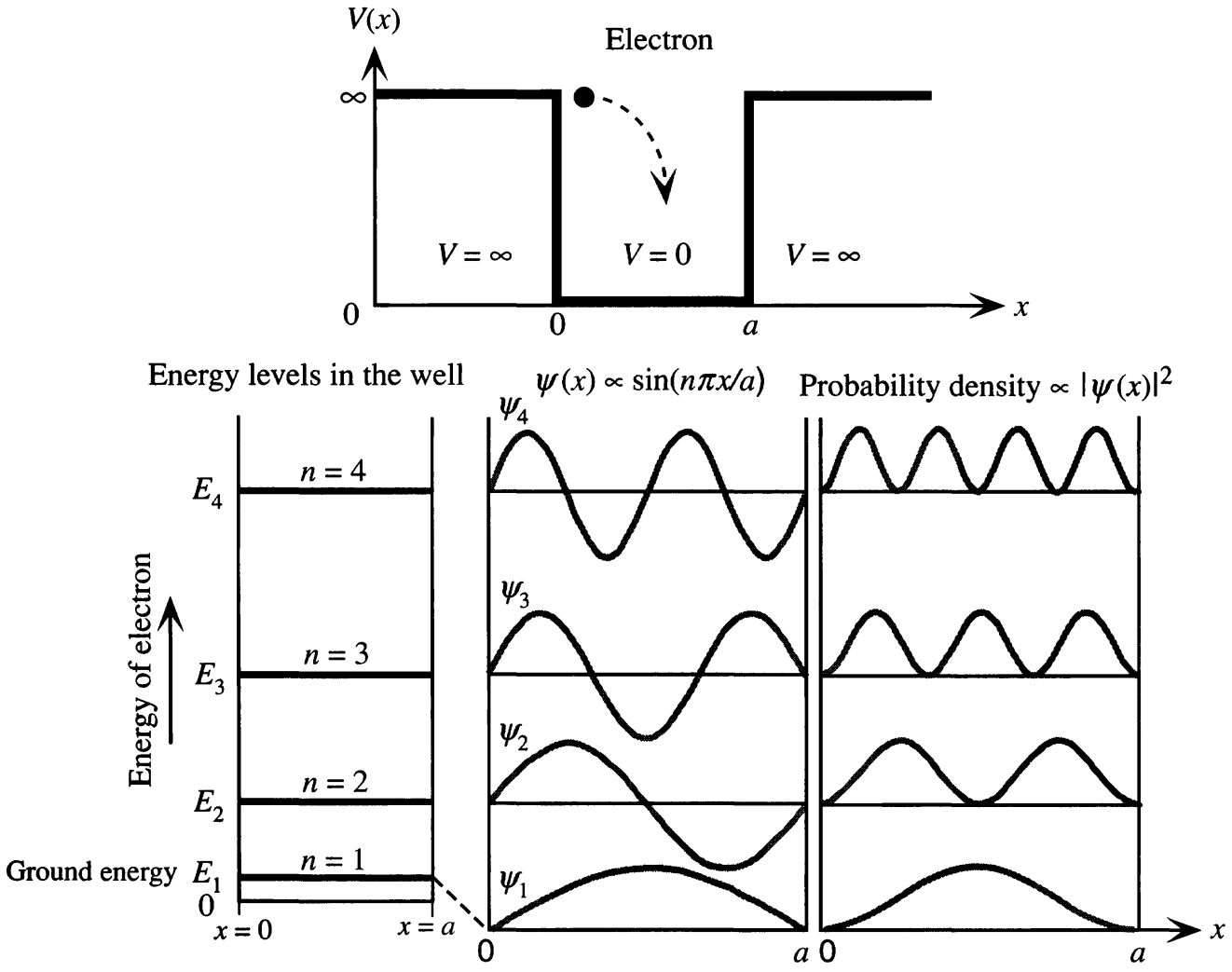


Figure 3.15 Electron in a one-dimensional infinite *PE* well.
The energy of the electron is quantized. Possible wavefunctions and the probability distributions for the electron are shown.

where k is some constant (to be determined) and substitute this in Equation 3.17 to find k. We first note that $\psi(0) = 0$; therefore, $B = -A$, so that

$$\psi(x) = A[\exp(jkx) - \exp(-jkx)] = 2Aj \sin kx \qquad [3.18]$$

We now substitute this into the Schrödinger Equation 3.17 to relate the energy E to k. Thus, Equation 3.17 becomes

$$-2Ajk^2(\sin kx) + \left(\frac{2m}{\hbar^2}\right)E(2Aj \sin kx) = 0$$

which can be rearranged to obtain the energy of the electron:

$$E = \frac{\hbar^2 k^2}{2m} \qquad [3.19]$$

Since the electron has no *PE* within the well, its total energy E is kinetic energy *KE*, and we can write

$$E = KE = \frac{p_x^2}{2m}$$

where p_x is its momentum. Comparing this with Equation 3.19, we see that the momentum of the electron must be

$$p_x = \pm\hbar k \qquad [3.20]$$

The momentum p_x may be in the $+x$ direction or the $-x$ direction (which is the reason for $\pm$), so the **average momentum** is actually zero, $p_{av} = 0$.

We have already seen this relationship, when we defined k as $2\pi/\lambda$ (wavenumber) for a free traveling wave. So the constant k here is a wavenumber-type quantity even though there is no distinct traveling wave. Its value is determined by the boundary condition at $x = a$ where $\psi = 0$, or

$$\psi(a) = 2Aj \sin ka = 0$$

The solution to $\sin ka = 0$ is simply $ka = n\pi$, where $n = 1, 2, 3, \ldots$ is an integer. We exclude $n = 0$ because it will result in $\psi = 0$ everywhere (no electron at all).

We notice immediately that k, and therefore the energy of the electron, can only have certain values; they are **quantized** by virtue of n being an integer. Here, n is called a **quantum number.** For each n, there is a special wavefunction

Wavefunction in infinite PE well

$$\psi_n(x) = 2Aj \sin\left(\frac{n\pi x}{a}\right) \qquad [3.21]$$

which is called an eigenfunction.[3] All ψ_n for $n = 1, 2, 3 \ldots$ constitute the eigenfunctions of the system. Each eigenfunction identifies a possible state for the electron. For each n, there is one special k value, $k_n = n\pi/a$, and hence a special energy value E_n, since

$$E_n = \frac{\hbar^2 k_n^2}{2m}$$

that is,

Electron energy in infinite PE well

$$E_n = \frac{\hbar^2(\pi n)^2}{2ma^2} = \frac{h^2 n^2}{8ma^2} \qquad [3.22]$$

The energies E_n defined by Equation 3.22 with $n = 1, 2, 3 \ldots$ are called **eigenenergies** of the system.

We still have not completely solved the problem, because A has yet to be determined. To find A, we use what is called the **normalization condition.** The total probability of finding the electron in the whole region $0 < x < a$ is unity, because we know the electron is somewhere in this region. Thus, $|\psi|^2\, dx$ summed between $x = 0$ and

[3] From the German meaning "characteristic function."

$x = a$ must be unity, or

$$\int_{x=0}^{x=a} |\psi(x)|^2 \, dx = \int_{x=0}^{x=a} \left| 2Aj \sin\left(\frac{n\pi x}{a}\right) \right|^2 dx = 1$$

Normalization condition

Carrying out the simple integration, we find

$$A = \left(\frac{1}{2a}\right)^{1/2}$$

The resulting wavefunction for the electron is thus

$$\psi_n(x) = j\left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right) \qquad [3.23]$$

We can now summarize the behavior of an electron in a one-dimensional *PE* well. Its wavefunction and energy, shown in Figure 3.15, are given by Equations 3.23 and 3.22, respectively. Both depend on the quantum number n. The energy of the electron increases with n^2, so the minimum energy of the electron corresponds to $n = 1$. This is called the **ground state,** and the energy of the ground state is the lowest energy the electron can possess. Note also that the energy of the electron in this potential well cannot be zero, even though the *PE* is zero. Thus, the electron always has *KE*, even when it is in the ground state.

The **node** of a wavefunction is defined as the point where $\psi = 0$ inside the well. It is apparent from Figure 3.15 that the ground wavefunction ψ_1 with the lowest energy has no nodes, ψ_2 has one node, ψ_3 has two nodes, and so on. Thus, the energy increases as the number of nodes increases in a wavefunction.

It may seem surprising that the energy of the electron is quantized; that is, that it can only have finite values, given by Equation 3.22. The electron cannot be made to take on any value of energy, as in the classical case. If the electron behaved like a particle, then an applied force F could impart any value of energy to it, because $F = dp/dt$ (Newton's second law), or $p = \int F dt$. By applying a force F for a time t, we can give the electron a *KE* of

$$E = \frac{p^2}{2m} = \left(\frac{1}{2}m\right)\left[\int F \, dt\right]^2$$

However, Equation 3.22 tells us that, in the microscopic world, the energy can only have quantized values. The two conflicting views can be reconciled if we consider the energy difference between two consecutive energy levels, as follows:

$$\Delta E = E_{n+1} - E_n = \frac{h^2(2n+1)}{8ma^2}$$

Energy separation in infinite PE well

As a increases to macroscopic dimensions, $a \to \infty$, the electron is completely free and $\Delta E \to 0$. Since $\Delta E = 0$, the energy of a completely free electron ($a = \infty$) is continuous. The energy of a confined electron, however, is quantized, and ΔE depends on the dimension (or size) of the potential well confining the electron.

In general, an electron will be "contained" in a spatial region of three dimensions, within which the *PE* will be lower (hence the confinement). We must then solve the

Schrödinger equation in three dimensions. The result is three quantum numbers that characterize the behavior of the electron.

Examination of the wavefunctions ψ_n in Figure 3.15 shows that these are either *symmetric* or *antisymmetric* with respect to the center of the well at $x = \frac{1}{2}a$. The symmetry of a wavefunction is called its **parity.** Whenever the potential energy function $V(x)$ exhibits symmetry about a certain point C, for example, about $x = \frac{1}{2}a$ in Figure 3.15, then the wavefunctions have either **even parity** (such as $\psi_1, \psi_3, \ldots$ that are symmetric) or have **odd parity** (such as $\psi_2, \psi_4, \ldots$ that are antisymmetric).

EXAMPLE 3.7 **ELECTRON CONFINED WITHIN ATOMIC DIMENSIONS** Consider an electron in an infinite potential well of size 0.1 nm (typical size of an atom). What is the ground energy of the electron? What is the energy required to put the electron at the third energy level? How can this energy be provided?

SOLUTION

The electron is confined in an infinite potential well, so its energy is given by

$$E_n = \frac{h^2 n^2}{8ma^2}$$

We use $n = 1$ for the ground level and $a = 0.1$ nm. Therefore,

$$E_1 = \frac{(6.6 \times 10^{-34}\ \text{J s})^2(1)^2}{8(9.1 \times 10^{-31}\ \text{kg})(0.1 \times 10^{-9}\ \text{m})^2} = 6.025 \times 10^{-18}\ \text{J} \quad \text{or} \quad 37.6\ \text{eV}$$

The frequency of the electron associated with this energy is

$$\omega = \frac{E}{\hbar} = \frac{6.025 \times 10^{-18}\ \text{J}}{1.055 \times 10^{-34}\ \text{J s}} = 5.71 \times 10^{16}\ \text{rad s}^{-1} \quad \text{or} \quad \nu = 9.092 \times 10^{15}\ \text{s}^{-1}$$

The third energy level E_3 is

$$E_3 = E_1 n^2 = (37.6\ \text{eV})(3)^2 = 338.4\ \text{eV}$$

The energy required to take the electron from 37.6 eV to 338.4 eV is 300.8 eV. This can be provided by a photon of exactly that energy; no less, and no more. Since the photon energy is $E = h\nu = hc/\lambda$, or

$$\lambda = \frac{hc}{E} = \frac{(6.6 \times 10^{-34}\ \text{J s})(3 \times 10^8\ \text{m s}^{-1})}{300.8\ \text{eV} \times 1.6 \times 10^{-19}\ \text{C}}$$

$$= 4.12\ \text{nm}$$

which is an X-ray photon.

EXAMPLE 3.8 **ENERGY OF AN APPLE IN A CRATE** Consider a macroscopic object of mass 100 grams (say, an apple) confined to move between two rigid walls separated by 1 m (say, a typical size of a large apple crate). What is the minimum speed of the object? What should the quantum number n be if the object is moving with a speed 1 m s^{-1}? What is the separation of the energy levels of the object moving with that speed?

SOLUTION

Since the object is within rigid walls, we take the *PE* outside the walls as infinite and use

$$E_n = \frac{h^2 n^2}{8ma^2}$$

to find the ground-level energy. With $n = 1$, $a = 1$ m, $m = 0.1$ kg, we have

$$E_1 = \frac{(6.6 \times 10^{-34}\ \text{J s})^2(1)^2}{8(0.1\ \text{kg})(1\ \text{m})^2} = 5.45 \times 10^{-67}\ \text{J} = 3.4 \times 10^{-48}\ \text{eV}$$

Since this is kinetic energy, $\frac{1}{2}mv_1^2 = E_1$, so the minimum speed is

$$v_1 = \sqrt{\frac{2E_1}{m}} = \sqrt{\frac{2(5.45 \times 10^{-67}\ \text{J})}{0.1\ \text{kg}}} = 3.3 \times 10^{-33}\ \text{m s}^{-1}$$

This speed cannot be measured by any instrument; therefore, for all practical purposes, the apple is at rest in the crate (a relief for the fruit grocer). The time required for the object to move a distance of 1 mm is 3×10^{29} s or 10^{21} years, which is more than the present age of the universe!

When the object is moving with a speed 1 m s^{-1},

$$KE = \frac{1}{2}mv^2 = \frac{1}{2}(0.1\ \text{kg})(1\ \text{m s}^{-1})^2 = 0.05\ \text{J}$$

This must be equal to $E_n = h^2n^2/8ma^2$ for some value of n

$$n = \left(\frac{8ma^2E_n}{h^2}\right)^{1/2} = \left[\frac{8(0.1\ \text{kg})(1\ \text{m})^2(0.05\ \text{J})}{(6.6 \times 10^{-34}\ \text{J s})^2}\right]^{1/2} = 3.03 \times 10^{32}$$

which is an enormous number. The separation between two energy levels corresponds to a change in n from 3.03×10^{32} to $3.03 \times 10^{32} + 1$. This is such a negligibly small change in n that for all practical purposes, the energy levels form a continuum. Thus,

$$\Delta E = E_{n+1} - E_n = \frac{h^2(2n+1)}{8ma^2}$$

$$= \frac{[(6.6 \times 10^{-34}\ \text{J s})^2(2 \times 3.03 \times 10^{32} + 1)]}{[8(0.1\ \text{kg})(1\ \text{m})^2]}$$

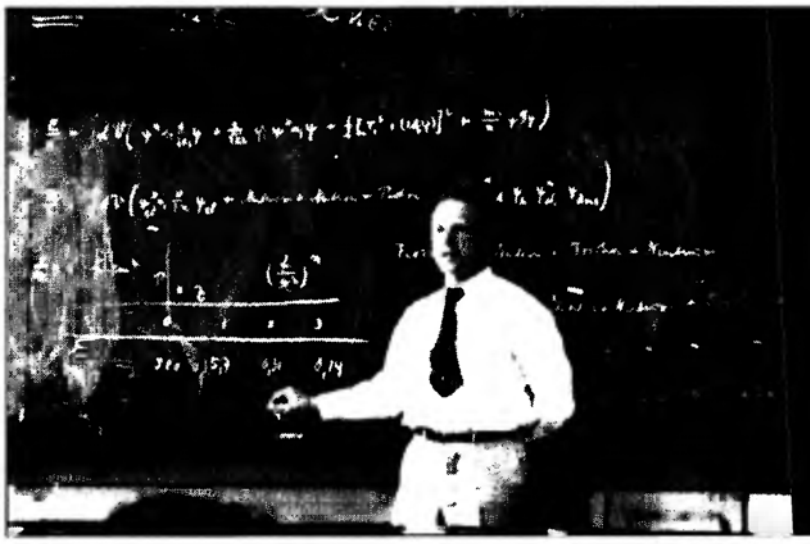
$$= 3.30 \times 10^{-34}\ \text{J} \quad \text{or} \quad 2.06 \times 10^{-15}\ \text{eV}$$

This energy separation is not detectable by any instrument. So for all practical purposes, the energy of the object changes continuously.

We see from this example that in the limit of large quantum numbers, quantum predictions agree with the classical results. This is the essence of **Bohr's correspondence principle.**

3.4 HEISENBERG'S UNCERTAINTY PRINCIPLE

The wavefunction of a free electron corresponds to a traveling wave with a single wavelength λ, as shown in Example 3.5. The traveling wave extends over all space, along all x, with the same amplitude, so the probability distribution function is uniform



Werner Heisenberg (1901–1976) received the Nobel prize in physics in 1932 for the uncertainty principle. This photo was apparently taken in 1936, while he was lecturing on quantum mechanics. "An expert is someone who knows some of the worst mistakes that can be made in his subject, and how to avoid them." W. Heisenberg.

SOURCE: AIP Emilio Segrè Visual Archives.

throughout the whole of space. The uncertainty Δx in the position of the electron is therefore infinite. Yet, the uncertainty Δp_x in the momentum of the electron is zero, because λ is well-defined, which means that we know p_x exactly from the de Broglie relationship, $p_x = h/\lambda$.

For an electron trapped in a one-dimensional infinite *PE* well, the wavefunction extends from $x = 0$ to $x = a$, so the uncertainty in the position of the electron is a. We know that the electron is within the well, but we cannot pinpoint with certainty exactly where it is. The momentum of the electron is either $p_x = \hbar k$ in the $+x$ direction or $-\hbar k$ in the $-x$ direction. The uncertainty Δp_x in the momentum is therefore $2\hbar k$; that is, $\Delta p_x = 2\hbar k$. For the ground-state wavefunction, which corresponds to $n = 1$, we have $ka = \pi$. Thus, $\Delta p_x = 2\hbar\pi/a$. Taking the product of the uncertainties in x and p, we get

$$(\Delta x)(\Delta p_x) = (a)\left(\frac{2\hbar\pi}{a}\right) = h$$

In other words, the product of the position and momentum uncertainties is simply h. This relationship is fundamental; and it constitutes a limit to our knowledge of the behavior of a system. *We cannot exactly and simultaneously know both the position and momentum of a particle along a given coordinate.* In general, if Δx and Δp_x are the respective uncertainties in the simultaneous measurement of the position and momentum of a particle along a particular coordinate (such as x), the **Heisenberg uncertainty principle** states that[4]

Heisenberg uncertainty principle for position and momentum

$$\Delta x\, \Delta p_x \gtrsim \hbar \qquad [3.24]$$

We are therefore forced to conclude that as previously stated, because of the wave nature of quantum mechanics, we are unable to determine exactly and simultaneously the position and momentum of a particle along a given coordinate. There will be an uncertainty Δx in the position and an uncertainty Δp_x in the momentum of the particle

[4] The Heisenberg uncertainty principle is normally written in terms of $\hbar$ rather than h. Further, in some physics texts, $\hbar$ in Equation 3.24 has a factor $\frac{1}{2}$ multiplying it.

and these uncertainties will be related by Heisenberg's uncertainty relationship in Equation 3.24.

These uncertainties are not in any way a consequence of the accuracy of a measurement or the precision of an instrument. Rather, they are the theoretical limits to what we can determine about a system. They are part of the quantum nature of the universe. In other words, even if we build the most perfectly engineered instrument to measure the position and momentum of a particle at one instant, we will still be faced with position and momentum uncertainties Δx and Δp_x such that $\Delta x\, \Delta p_x > \hbar$.

There is a similar uncertainty relationship between the uncertainty ΔE in the energy E (or angular frequency ω) of the particle and the time duration Δt during which it possesses the energy (or during which its energy is measured). We know that the kx part of the wave leads to the uncertainty relation $\Delta x\, \Delta p_x > \hbar$ or $\Delta x\, \Delta k \geq 1$. By analogy we should expect a similar relationship for the ωt part, or $\Delta\omega\, \Delta t \geq 1$. This hypothesis is true, and since $E = \hbar\omega$, we have the uncertainty relation for the particle energy and time:

Heisenberg uncertainty principle for energy and time

$$\Delta E\, \Delta t \gtrsim \hbar \qquad [3.25]$$

Note that the uncertainty relationships in Equations 3.24 and 3.25 have been written in terms of $\hbar$, rather than h, as implied by the electron in an infinite potential energy well ($\Delta x\, \Delta p_x \geq h$). In general there is also a numerical factor of $\frac{1}{2}$ multiplying $\hbar$ in Equations 3.24 and 3.25 which comes about when we consider a Gaussian spread for all possible position and momentum values. The proof is not presented here, but can be found in advanced quantum mechanics books.

It is important to note that the uncertainty relationship applies only when the position and momentum are measured in the same direction (such as the x direction). On the other hand, the exact momentum, along, say, the y direction and the exact position, along, say, the x direction can be determined exactly, since $\Delta x\, \Delta p_y$ need not satisfy the Heisenberg uncertainty relationship (in other words, $\Delta x\, \Delta p_y$ can be zero).

EXAMPLE 3.9

THE MEASUREMENT TIME AND THE FREQUENCY OF WAVES: AN ANALOGY WITH $\Delta E\, \Delta t \geq \hbar$

Consider the measurement of the frequency of a sinusoidal wave of frequency 1000 Hz (or cycles/s). Suppose we can only measure the number of cycles to an accuracy of 1 cycle, because we need to receive a whole cycle to record it as one complete cycle. Then, in a time interval of $\Delta t = 1$ s, we will register 1000 ± 1 cycles. The uncertainty Δf in the frequency is 1 cycle/1 s or 1 Hz. If Δt is 2 s, we will measure 2000 ± 1 cycles, and the uncertainty Δf will be 1 cycle/2 s or $\frac{1}{2}$ cycle/s or $\frac{1}{2}$ Hz. Thus, Δf decreases with Δt.

Suppose that in a time interval Δt, we measure $N \pm 1$ cycles. Since the uncertainty is 1 cycle in a time interval Δt, the uncertainty in f will be

$$\Delta f = \frac{(1 \text{ cycle})}{\Delta t} = \frac{1}{\Delta t} \text{ Hz}$$

Since $\omega = 2\pi f$, we have

$$\Delta\omega\, \Delta t = 2\pi$$

In quantum mechanics, under steady-state conditions, an object has a time-oscillating wavefunction with a frequency ω which is related to its energy E by $\omega = E/\hbar$ (see Equation 3.15).

Substituting this into the previous relationship gives

$$\Delta E \, \Delta t = h$$

The uncertainty in the energy of a quantum object is therefore related, in a fundamental way, to the time duration during which the energy is observed. Notice that we again have h, as for $\Delta x \, \Delta p_x = h$, though the quantum mechanical uncertainty relationship in Equation 3.25 has $\hbar$.

EXAMPLE 3.10 **THE UNCERTAINTY PRINCIPLE ON THE ATOMIC SCALE** Consider an electron confined to a region of size 0.1 nm, which is the typical dimension of an atom. What will be the uncertainty in its momentum and hence its kinetic energy?

SOLUTION

We apply the Heisenberg uncertainty relationship, $\Delta x \, \Delta p_x \approx \hbar$, or

$$\Delta p_x \approx \frac{\hbar}{\Delta x} = \frac{1.055 \times 10^{-34} \text{ J s}}{0.1 \times 10^{-9} \text{ m}} = 1.055 \times 10^{-24} \text{ kg m s}^{-1}$$

The uncertainty in the velocity is therefore

$$\Delta v = \frac{\Delta p_x}{m_e} = \frac{1.055 \times 10^{-24} \text{ kg m s}^{-1}}{9.1 \times 10^{-31} \text{ kg}} = 1.16 \times 10^{6} \text{ m s}^{-1}$$

We can take this uncertainty to represent the order of magnitude of the actual speed. The kinetic energy associated with this momentum is

$$KE = \frac{\Delta p_x^2}{2m_e} = \frac{(1.055 \times 10^{-24} \text{ kg m s}^{-1})^2}{2(9.1 \times 10^{-31} \text{ kg})}$$

$$= 6.11 \times 10^{-19} \text{ J} \quad \text{or} \quad 3.82 \text{ eV}$$

EXAMPLE 3.11 **THE UNCERTAINTY PRINCIPLE WITH MACROSCOPIC OBJECTS** Estimate the minimum velocity of an apple of mass 100 g confined to a crate of size 1 m.

SOLUTION

Taking the uncertainty in the position of the apple as 1 m, the apple is somewhere in the crate,

$$\Delta p_x \approx \frac{\hbar}{\Delta x} = \frac{1.05 \times 10^{-34} \text{ J s}}{1 \text{ m}} = 1.05 \times 10^{-34} \text{ kg m s}^{-1}$$

So the minimum uncertainty in the velocity is

$$\Delta v_x = \frac{\Delta p_x}{m} = \frac{1.05 \times 10^{-34} \text{ kg m s}^{-1}}{0.1 \text{ kg}} = 1.05 \times 10^{-33} \text{ m s}^{-1}$$

The quantum nature of the universe implies that the apple in the crate is moving with a velocity on the order of 10^{-33} m s^{-1}. This cannot be measured by any instrument; indeed, it would take the apple $\sim 10^{19}$ years to move an atomic distance of 0.1 nm.

3.5 TUNNELING PHENOMENON: QUANTUM LEAK

To understand the tunneling phenomenon, let us examine the thrilling events experienced by the roller coaster shown in Figure 3.16a. Consider what the roller coaster can do when released from rest at a height A. The conservation of energy means that the carriage can reach B and at most C, but certainly not beyond C and definitely not D and E. Classically, there is no possible way the carriage will reach E at the other side of the potential barrier D. An extra energy corresponding to the height difference, $D - A$, is needed. Anyone standing at E will be quite safe. Ignoring frictional losses, the roller coaster will go back and forth between A and C.

Now, consider an analogous event on an atomic scale. An electron moves with an energy E in a region $x < 0$ where the potential energy PE is zero; therefore, E is solely kinetic energy. The electron then encounters a potential barrier of "height" V_o, which

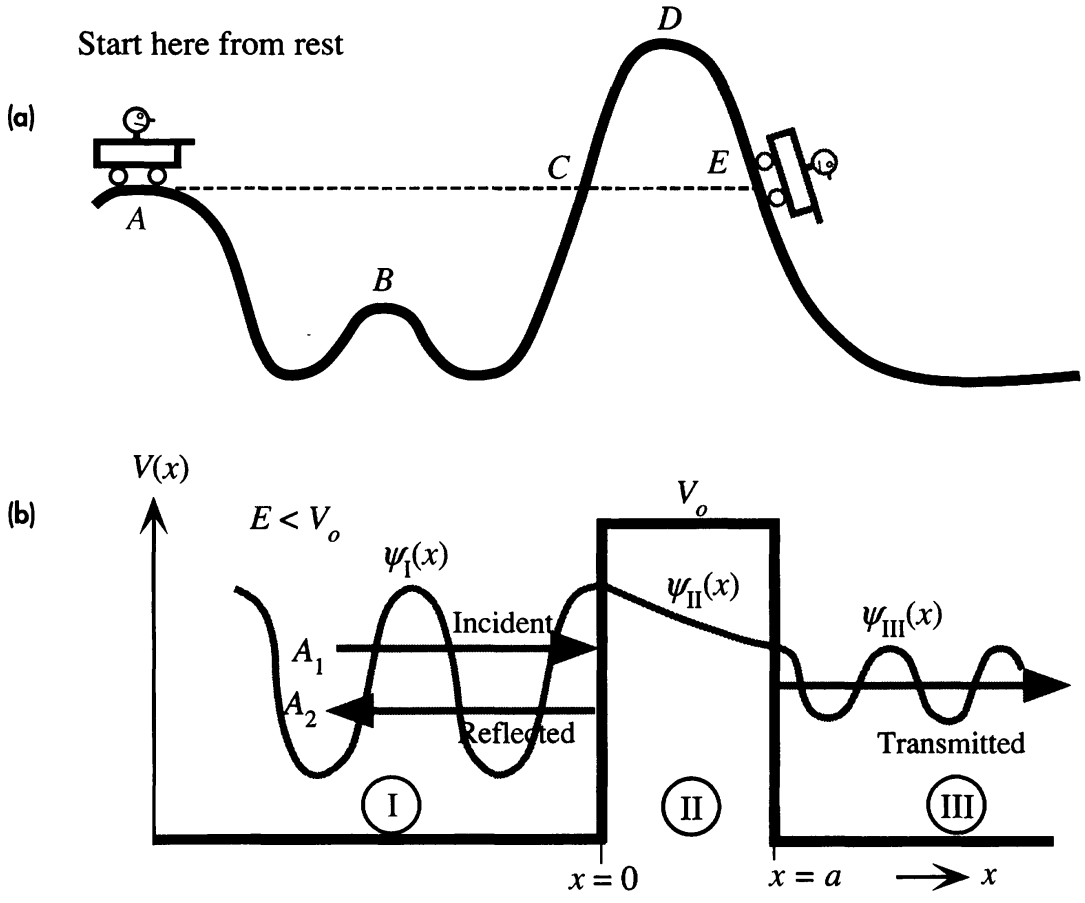


Figure 3.16

(a) The roller coaster released from A can at most make it to C, but not to E. Its PE at A is less than the PE at D. When the car is at the bottom, its energy is totally KE. CD is the energy barrier that prevents the car from making it to E. In quantum theory, on the other hand, there is a chance that the car could tunnel (leak) through the potential energy barrier between C and E and emerge on the other side of the hill at E.

(b) The wavefunction for the electron incident on a potential energy barrier (V_o). The incident and reflected waves interfere to give $\psi_I(x)$. There is no reflected wave in region III. In region II, the wavefunction decays with x because $E < V_o$.

is greater than E at $x = 0$. The extent (width) of the potential barrier is a. On the other side of the potential barrier, $x > a$, the *PE* is again zero. What will the electron do? Classically, just like the roller coaster, the electron should bounce back and thus be confined to the region $x < 0$, because its total energy E is less than V_o. In the quantum world, however, there is a distinct possibility that the electron will "tunnel" through the potential barrier and appear on the other side; it will leak through.

To show this, we need to solve the Schrödinger equation for the present choice of $V(x)$. Remember that the only way the Schrödinger equation will have the solution $\psi(x) = 0$ is if the *PE* is infinite, that is, $V = \infty$. Therefore, within any zero or finite *PE* region, there will always be a solution $\psi(x)$ and there always will be some probability of finding the electron.

We can divide the electron's space into three regions, I, II, and III, as indicated in Figure 3.16b. We can then solve the Schrödinger equation for each region, to obtain three wavefunctions $\psi_{\mathrm{I}}(x)$, $\psi_{\mathrm{II}}(x)$, and $\psi_{\mathrm{III}}(x)$. In regions I and III, $\psi(x)$ must be traveling waves, as there is no *PE* (the electron is free and moving with a kinetic energy E). In zone II, however, $E - V_o$ is negative, so the general solution of the Schrödinger equation is the sum of an exponentially decaying function and an exponentially increasing function. In other words,

$$\psi_{\mathrm{I}}(x) = A_1 \exp(jkx) + A_2 \exp(-jkx) \qquad [3.26a]$$

$$\psi_{\mathrm{II}}(x) = B_1 \exp(\alpha x) + B_2 \exp(-\alpha x) \qquad [3.26b]$$

$$\psi_{\mathrm{III}}(x) = C_1 \exp(jkx) + C_2 \exp(-jkx) \qquad [3.26c]$$

are the wavefunctions in which

$$k^2 = \frac{2mE}{\hbar^2} \qquad [3.27]$$

and

$$\alpha^2 = \frac{2m(V_o - E)}{\hbar^2} \qquad [3.28]$$

Both k^2 and α^2, and hence k and α, in Equations 3.26a to c are positive numbers. This means that $\exp(jkx)$ and $\exp(-jkx)$ represent traveling waves in opposite directions, and $\exp(-\alpha x)$ and $\exp(\alpha x)$ represent an exponential decay and rise, respectively. We see that in region I, $\psi_{\mathrm{I}}(x)$ consists of the incident wave $A_1 \exp(jkx)$ in the $+x$ direction, and a reflected wave $A_2 \exp(-jkx)$, in the $-x$ direction. Furthermore, because the electron is traveling toward the right in region III, there is no reflected wave, so $C_2 = 0$.

We must now apply the boundary conditions and the normalization condition to determine the various constants A_1, A_2, B_1, B_2, and C_1. In other words, we must match the three waveforms in Equations 3.26a to c at their boundaries ($x = 0$ and $x = a$) so that they form a continuous single-valued wavefunction. With the boundary conditions enforced onto the wavefunctions $\psi_{\mathrm{I}}(x)$, $\psi_{\mathrm{II}}(x)$, and $\psi_{\mathrm{III}}(x)$, all the constants can be determined in terms of the amplitude A_1 of the incoming wave. The relative probability that the electron will tunnel from region I through to III is defined as the **transmission**

coefficient *T*, and this depends very strongly on both the relative *PE* barrier height $(V_o - E)$ and the width a of the barrier. The final result that comes out from a tedious application of the boundary conditions is

$$T = \frac{|\psi_{III}(x)|^2}{|\psi_I(\text{incident})|^2} = \frac{C_1^2}{A_1^2} = \frac{1}{1 + D\sinh^2(\alpha a)} \qquad [3.29]$$

Probability of tunneling

where

$$D \doteq \frac{V_o^2}{4E(V_o - E)} \qquad [3.30]$$

and α is the rate of decay of $\psi_{II}(x)$ as expressed in Equation 3.28. For a wide or high barrier, using $\alpha a \gg 1$ in Equation 3.29 and $\sinh(\alpha a) \approx \frac{1}{2}\exp(\alpha a)$, we can deduce

$$T = T_o \exp(-2\alpha a) \qquad [3.31]$$

Probability of tunneling through

where

$$T_o = \frac{16E(V_o - E)}{V_o^2} \qquad [3.32]$$

By contrast, the relative probability of reflection is determined by the ratio of the square of the amplitude of the reflected wave to that of the incident wave. This quantity is the **reflection coefficient *R*,** which is given by

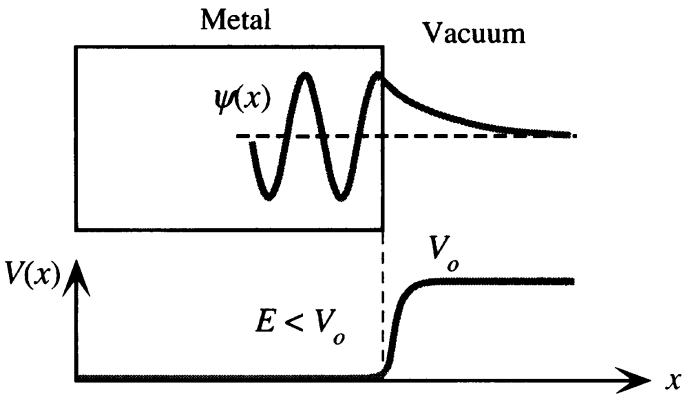
$$R = \frac{A_2^2}{A_1^2} = 1 - T \qquad [3.33]$$

Reflection coefficient

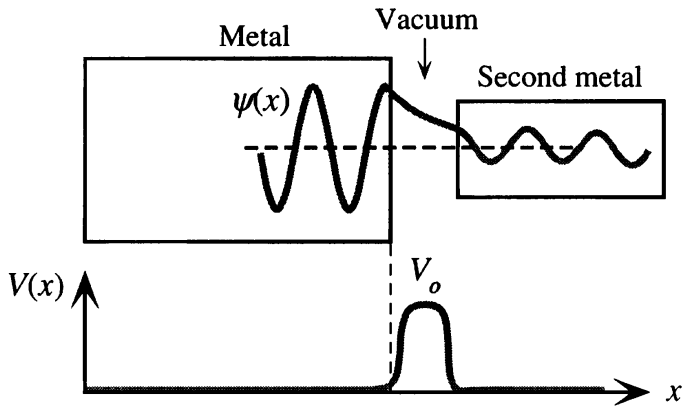
We can now summarize the entire tunneling affair as follows. When an electron encounters a potential energy barrier of height V_o greater than its energy E, there is a finite probability that it will leak through that barrier. This probability depends sensitively on the energy and width of the barrier. For a wide potential barrier, the probability of tunneling is proportional to $\exp(-2\alpha a)$, as in Equation 3.31. The wider or higher the potential barrier, the smaller the chance of the electron tunneling.

One of the most remarkable technological uses of the tunneling effect is in the scanning tunneling microscope (STM), which elegantly maps out the surfaces of solids. A conducting probe is brought so close to the surface of a solid that electrons can tunnel from the surface of the solid to the probe, as illustrated in Figure 3.17. When the probe is far removed, the wavefunction of an electron decays exponentially outside the material, by virtue of the potential energy barrier being finite (the work function is ~10 eV). When the probe is brought very close to the surface, the wavefunction penetrates into the probe and, as a result, the electron can tunnel from the material into the probe. Without an applied voltage, there will be as many electrons tunneling from the material to the probe as there are going in the opposite direction from the probe to the material, so the net current will be zero.

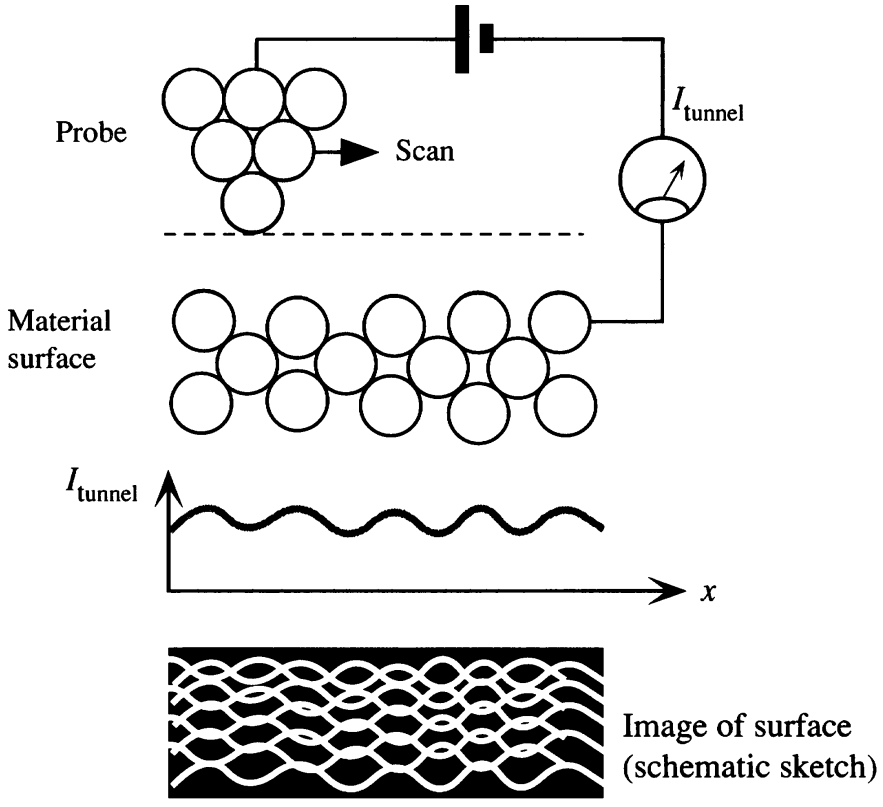
On the other hand, if a positive bias is applied to the probe with respect to the material, as shown in Figure 3.17, an electron tunneling from the material to the probe will see a lower potential barrier than one tunneling from the probe to the material. Consequently, there will be a net current from the probe to the material and this current



(a) The wavefunction decays exponentially as we move away from the surface because the *PE* outside the metal is V_o and the energy of the electron, $E < V_o$.



(b) If we bring a second metal close to the first metal, then the wavefunction can penetrate into the second metal. The electron can tunnel from the first metal to the second.



(c) The principle of the scanning tunneling microscope. The tunneling current depends on $\exp(-2\alpha a)$ where a is the distance of the probe from the surface of the specimen and α is a constant.

Figure 3.17

will depend very sensitively on the separation a of the probe from the surface, by virtue of Equation 3.31.

Because the tunneling current is extremely sensitive to the width of the potential barrier, the tunneling current is essentially dominated by electrons tunneling to the probe atom nearest to the surface. Thus, the probe tip has an atomic dimension. By scanning the surface of the material with the probe and recording the tunneling current

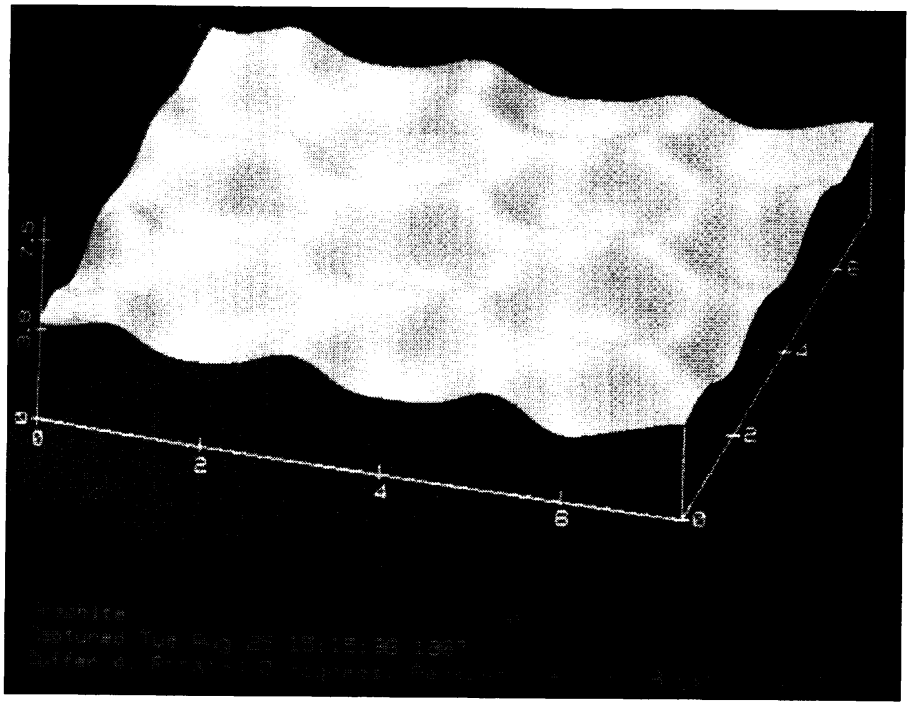
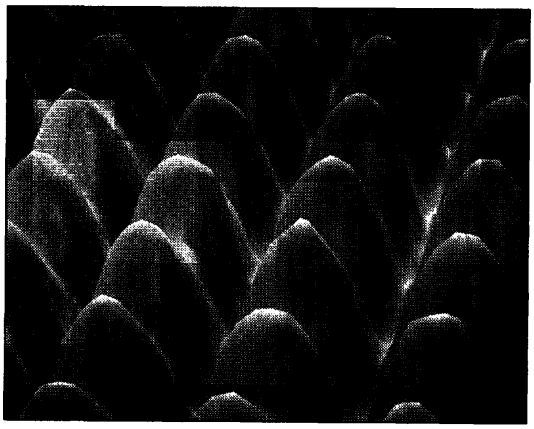


Figure 3.18 Scanning tunneling microscope (STM) image of a graphite surface where contours represent electron concentrations within the surface, and carbon rings are clearly visible. The scale is in 2 Å.
SOURCE: Courtesy of Veeco Instruments, Metrology Division, Santa Barbara, CA.

the user can map out the surface topology of the material with a resolution comparable to the atomic dimension. The probe motion along the surface, and also perpendicular to the surface, is controlled by piezoelectric transducers to provide sufficiently small and smooth displacements. Figure 3.18 shows an STM image of a graphite surface, on which the hexagonal carbon rings can be clearly seen. Notice that the scale is 0.2 nm (2 Å). The contours in the image actually represent electron concentrations within the surface since it is the electrons that tunnel from the graphite surface to the probe tip. The astute reader will notice that not all the carbon atoms in a hexagonal ring are at the same height; three are higher and three are lower. The reason is that the exact electron concentration on the surface is also influenced by the second layer of atoms underneath the top layer. The overall effect makes the electron concentration

STM's inventors Gerd Binning (right) and Heinrich Rohrer (left), at IBM Zurich Research Laboratory with one of their early devices. They won the 1986 Nobel prize for the STM.
SOURCE: Courtesy of IBM Zurich Research Laboratory.



An STM image of a Ni (110) surface.
SOURCE: Courtesy of IBM.

change (alternate) from one atomic site to a neighboring site within the hexagonal rings. STM was invented by Gerd Binning and Heinrich Rohrer at the IBM Research Laboratory in Zurich, for which they were awarded the 1986 Nobel prize.[5]

EXAMPLE 3.12 **TUNNELING CONDUCTION THROUGH METAL-TO-METAL CONTACTS** Consider two copper wires separated only by their surface oxide layer (CuO). Classically, since the oxide layer is an insulator, no current should be possible through the two copper wires. Suppose that for the conduction ("free") electrons in copper, the surface oxide layer looks like a square potential energy barrier of height 10 eV. Consider an oxide layer thickness of 5 nm and evaluate the transmission coefficient for conduction electrons in copper, which have a kinetic energy of about 7 eV. What will be the transmission coefficient if the oxide barrier is 1 nm?

SOLUTION

We can calculate α from

$$\alpha = \left[\frac{2m(V_o - E)}{\hbar^2}\right]^{1/2}$$

$$= \left[\frac{2(9.1 \times 10^{-31}\,\text{kg})(10\,\text{eV} - 7\,\text{eV})(1.6 \times 10^{-19}\,\text{J/eV})}{(1.05 \times 10^{-34}\,\text{J s})^2}\right]^{1/2}$$

$$= 8.9 \times 10^9\,\text{m}^{-1}$$

so that

$$\alpha a = (8.9 \times 10^9\,\text{m}^{-1})(5 \times 10^{-9}\,\text{m}) = 44.50$$

Since this is greater than unity, we use the wide-barrier transmission coefficient in Equation 3.31.

Now,

$$T_o = \frac{16E(V_o - E)}{V_o^2} = \frac{16(7\,\text{eV})(10\,\text{eV} - 7\,\text{eV})}{(10\,\text{eV})^2} = 3.36$$

Thus,

$$T = T_o \exp(-2\alpha a)$$

$$= 3.36 \exp[-2(8.9 \times 10^9\,\text{m}^{-1})(5 \times 10^{-9}\,\text{m})] = 3.36\exp(-89)$$

$$\approx 7.4 \times 10^{-39}$$

an incredibly small number.

With $a = 1$ nm,

$$T = 3.36 \exp[-2(8.9 \times 10^9\,\text{m}^{-1})(1 \times 10^{-9}\,\text{m})]$$

$$= 3.36 \exp(-17.8) \approx 6.2 \times 10^{-8}$$

Notice that reducing the layer thickness by five times increases the transmission probability by 10^{31}! Small changes in the barrier width lead to enormous changes in the transmission

[5] The IBM Research Laboratory in Zurich, Switzerland, received both the 1986 and the 1987 Nobel prizes. The first was for the scanning tunneling microscope by Gerd Binning and Heinrich Rohrer. The second was awarded to Georg Bednorz and Alex Müller for the discovery of high-temperature superconductors which we will examine in Chapter 8.

probability. We should note that when a voltage is applied across the two wires, the potential energy height is altered (PE = charge × voltage), which results in a large increase in the transmission probability and hence results in a current.

EXAMPLE 3.13

SIGNIFICANCE OF A SMALL $\hbar$ Estimate the probability that a roller coaster carriage that weighs 100 kg released from point A in Figure 3.16a from a height at 10 m can reach point E over a hump that is 15 m high and 10 m wide. What will this probability be in a universe where $\hbar \approx 10$ kJ s?

SOLUTION

The total energy of the carriage at height A is

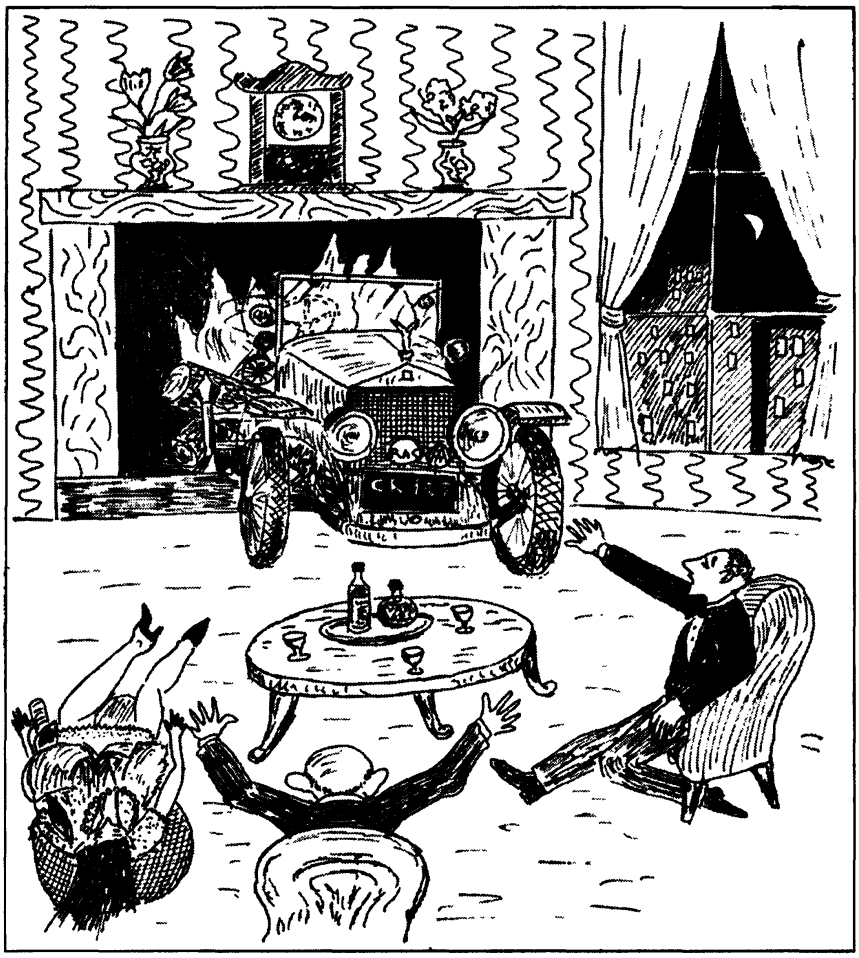
$$E = PE = mg(\text{height}) = (100\text{ kg})(10\text{ m s}^{-2})(10\text{ m}) = 10^4\text{ J}$$

Suppose that as a first approximation, we can approximate the hump as a square hill of height 15 m and width 10 m. The PE required to reach the peak would be

$$V_o = mg(\text{height}) = (100\text{ kg})(10\text{ m s}^{-2})(15\text{ m}) = 1.5 \times 10^4\text{ J}$$

Applying this, we have

$$\alpha^2 = \frac{2m(V_o - E)}{\hbar^2} = \frac{2(100\text{ kg})(1.5 \times 10^4\text{ J} - 10^4\text{ J})}{(1.05 \times 10^{-34}\text{ J s})^2} = 9.07 \times 10^{73}\text{ m}^{-2}$$



"Just like the good old ghost of the middle ages." In a world where $\hbar$ is of the order of unity, one can expect tunneling surprises.

SOURCE: George Gamow, *Mr. Tompkins in Paperback*, Cambridge, England, University Press, 1965, p. 96. Used with permission.

and so

$$\alpha = 9.52 \times 10^{36}\ \text{m}^{-1}$$

With $a = 10$ m, we have $\alpha a \gg 1$, so we can use the wide-barrier tunneling equation,

$$T = T_o \exp(-2\alpha a)$$

where

$$T_o = \frac{16[E(V_o - E)]}{V_o^2} = 3.56$$

Thus,

$$T = 3.56 \exp[-2(9.52 \times 10^{36}\ \text{m}^{-1})(10\ \text{m})] = 3.56 \exp(-1.9 \times 10^{38})$$

which is a fantastically small number, indicating that it is impossible for the carriage to tunnel through the hump.

Suppose that $\hbar \approx 10$ kJ s. Then

$$\alpha^2 = \frac{2m(V_o - E)}{\hbar^2} = \frac{2(100\ \text{kg})(1.5 \times 10^4\ \text{J} - 10^4\ \text{J})}{(10^4\ \text{J s})^2} = 0.01\ \text{m}^{-2}$$

so that $\alpha = 0.1\ \text{m}^{-1}$. Clearly, $\alpha a = 1$, so we must use

$$T = [1 + D \sinh^2(\alpha a)]^{-1}$$

where

$$D = \frac{V_o^2}{[4E(V_o - E)]} = 1.125$$

Thus,

$$T = [1 + 1.125 \sinh^2(1)]^{-1} = 0.39$$

Thus, after three goes, the carriage would tunnel to the other side (giving the person standing at E the shock of his life).

3.6 POTENTIAL BOX: THREE QUANTUM NUMBERS

To examine the properties of a particle confined to a region of space, we take a three-dimensional space with a volume marked by a, b, c along the x, y, z axes. The PE is zero ($V = 0$) inside the space and is infinite on the outside, as illustrated in Figure 3.19. This is a three-dimensional potential energy well. The electron essentially lives in the "box." What will the behavior of the electron be in this box? In this case we need to solve the three-dimensional version of the Schrödinger equation,[6] which is

Schrödinger equation in three dimensions

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \qquad [3.34]$$

[6] The term $\partial\psi/\partial x$ simply means differentiating $\psi(x, y, z)$ with respect to x while keeping y and z constant, just like $d\psi/dx$ in one dimension.

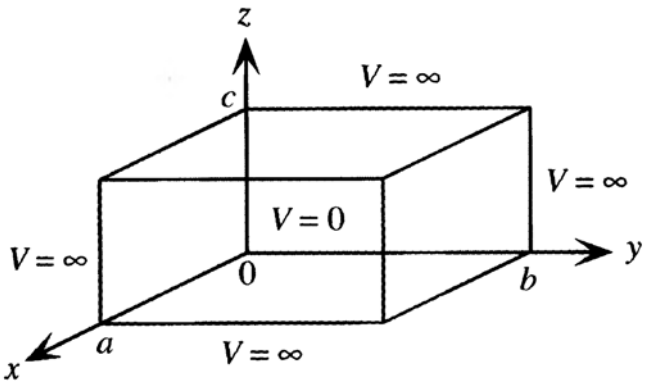


Figure 3.19 Electron confined in three dimensions by a three-dimensional infinite *PE* box.
Everywhere inside the box, $V = 0$, but outside, $V = \infty$. The electron cannot escape from the box.

with $V = 0$ in $0 < x < a$, $0 < y < b$, and $0 < z < c$, and V infinite outside. We can try to solve this by separating the variables via $\psi(x, y, z) = \psi_x(x)\,\psi_y(y)\,\psi_z(z)$. Substituting this back into Equation 3.34, we can obtain three ordinary differential equations, each just like the one for the one-dimensional potential well. Having found $\psi_x(x)$, $\psi_y(y)$, and $\psi_z(z)$ we know that the total wavefunction is simply the product,

$$\psi(x, y, z) = A \sin(k_x x) \sin(k_y y) \sin(k_z z) \qquad [3.35]$$

where k_x, k_y, k_z, and A are constants to be determined. We can then apply the boundary conditions at $x = a$, $y = b$, and $z = c$ to determine the constants k_x, k_y, and k_z in the same way we found k for the one-dimensional potential well. If $\psi(x, y, z) = 0$ at $x = a$, then k_x will be quantized via

$$k_x a = n_1 \pi$$

where n_1 is a quantum number, $n_1 = 1, 2, 3, \ldots$. Similarly, if $\psi(x, y, z) = 0$ at $y = b$ and $z = c$, then k_y and k_z will be quantized, so that, overall, we will have

$$k_x = \frac{n_1 \pi}{a} \qquad k_y = \frac{n_2 \pi}{b} \qquad k_z = \frac{n_3 \pi}{c} \qquad [3.36]$$

where n_1, n_2, and n_3 are quantum numbers, each of which can be any integer except zero.

We notice immediately that in three dimensions, we have three quantum numbers n_1, n_2, and n_3 associated with $\psi_x(x)$, $\psi_y(y)$, and $\psi_z(z)$. The eigenfunctions of the electron, denoted by the quantum numbers n_1, n_2, and n_3, are now given by

Electron wavefunction in infinite PE well

$$\psi_{n_1 n_2 n_3}(x, y, z) = A \sin\left(\frac{n_1 \pi x}{a}\right) \sin\left(\frac{n_2 \pi y}{b}\right) \sin\left(\frac{n_3 \pi z}{c}\right) \qquad [3.37]$$

Notice that these consist of the products of infinite one-dimensional *PE* well-type wavefunctions, one for each dimension, and each has its own quantum number n. Each possible eigenfunction can be labeled a **state** for the electron. Thus, ψ_{111} and ψ_{121} are two possible states.

To find the constant A in Equation 3.37, we need to use the normalization condition that $|\psi_{n_1 n_2 n_3}(x, y, z)|^2$ integrated over the volume of the box must be unity,

since the electron is somewhere in the box. The result for a square box is $A = (2/a)^{3/2}$.

We can find the energy of the electron by substituting the wavefunction in Equation 3.35 into the Schrödinger Equation 3.34. The energy as a function of k_x, k_y, k_z is then found to be

$$E = E(k_x, k_y, k_z) = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)$$

which is quantized by virtue of k_x, k_y, and k_z being quantized. We can write this energy in terms of n_1^2, n_2^2, and n_3^2 by using Equation 3.36, as follows:

$$E_{n_1 n_2 n_3} = \frac{h^2}{8m}\left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2}\right)$$

For a square box for which $a = b = c$, the energy is

Electron energy in infinite PE box

$$E_{n_1 n_2 n_3} = \frac{h^2\left(n_1^2 + n_2^2 + n_3^2\right)}{8ma^2} = \frac{h^2 N^2}{8ma^2} \qquad [3.38]$$

where $N^2 = (n_1^2 + n_2^2 + n_3^2)$, which can only have certain integer values. It is apparent that the energy now depends on three quantum numbers. Our conclusion is that in three dimensions, we have three quantum numbers, each one arising from boundary conditions along one of the coordinates. They quantize the energy of the electron via Equation 3.38 and its momentum in a particular direction, such as, $p_x = \pm\hbar k_x = \pm(hn_1/2a)$, though the average momentum is zero.

The lowest energy for the electron is obviously equal to E_{111}, not zero. The next energy level corresponds to E_{211}, which is the same as E_{121} and E_{112}, so there are three states (*i.e.*, ψ_{211}, ψ_{121}, ψ_{112}) for this energy. The number of states that have the same energy is termed the **degeneracy** of that energy level. The second energy level E_{211} is thus **three-fold degenerate.**

EXAMPLE 3.14 **NUMBER OF STATES WITH THE SAME ENERGY** How many states (eigenfunctions) are there at energy level E_{443} for a square potential energy box?

SOLUTION

This energy level corresponds to $n_1 = 4$, $n_2 = 4$, and $n_3 = 3$, but the energy depends on

$$N^2 = n_1^2 + n_2^2 + n_3^2 = 4^2 + 4^2 + 3^2 = 41$$

via Equation 3.38. As long as $N^2 = 41$ for any choice of (n_1, n_2, n_3), not just (4, 4, 3), the energy will be the same.

The value $N^2 = 41$ can be obtained from (4, 4, 3), (4, 3, 4), and (3, 4, 4) as well as (6, 2, 1), (6, 1, 2), (2, 6, 1), (2, 1, 6), (1, 6, 2), and (1, 2, 6). There are thus three states from (4, 4, 3) combinations and six from (6, 2, 1) combinations, giving nine possible states, each with a distinct wavefunction, $\psi_{n_1 n_2 n_3}$. However, all these $\psi_{n_1 n_2 n_3}$ for the electron have the same energy E_{443}.