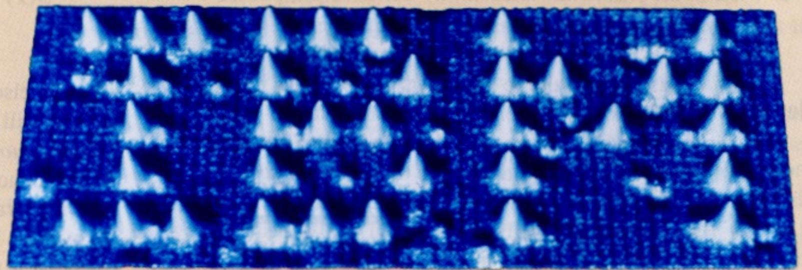
41 One-Dimensional Quantum Mechanics



An example of atomic engineering. Thirty-five xenon atoms have been manipulated into position with the probe tip of a scanning tunneling microscope.

► Looking Ahead

The goal of Chapter 41 is to understand and apply the essential ideas of quantum mechanics. In this chapter you will learn to:

- Use a strategy for finding and interpreting wave functions.
- Draw wave functions with appropriate shapes.
- Use potential-energy functions to make quantum-mechanical models.
- Understand and use several important quantum-mechanical models.
- Calculate the probability of quantum-mechanical tunneling.

◄ Looking Back

Quantum mechanics will be developed around two fundamental ideas: energy diagrams and wave functions. A review of energy diagrams in Chapter 10 is especially important. Please review:

- Section 10.7 Energy diagrams.
- Sections 39.4 and 39.5 Matter waves and the Bohr model of quantization.
- Sections 40.3 and 40.4 Wave functions and normalization.

Quantum mechanics is not just for physicists any more. It is now an essential tool in the design of semiconductor devices such as diode lasers. Whole new classes of devices, called *quantum-well devices,* have been designed and built to exploit the quantization of energy levels. We will look at some examples in this chapter.

Also at the cutting edge of engineering science is the design and manufacture of *nanostructures*—small machines or other devices only a few hundred nanometers in size. Many scientists and engineers envision a day in the near future when nanostructures will be constructed literally atom by atom. Quantum effects will be important in devices this small. This photograph—of a structure built by scientists at IBM's research laboratory by moving xenon atoms around on a metal surface—shows an early example of "atomic engineering."

Our goal for this chapter is to introduce the essential ideas of quantum mechanics. Although the real world is three-dimensional, we will limit our study of quantum mechanics to one dimension. This will allow us to focus on the fundamental concepts of quantum physics without becoming overwhelmed by mathematical complications. We will discuss some of the aspects of finding and using wave functions, then look at several applications of quantum mechanics. We'll conclude this chapter with a look at a phenomenon called *quantum-mechanical tunneling,* one of the more startling aspects of quantum physics.

41.1 Schrödinger's Equation: The Law of Psi

In the winter of 1925, just before Christmas, the Austrian physicist Erwin Schrödinger gathered together a few books and headed off to a villa in the Swiss Alps. He had recently learned of de Broglie's 1924 suggestion that matter has wave-like properties, and he wanted some time free from distractions to think about it. Before the trip was over, Schrödinger had discovered the law of quantum mechanics.

Schrödinger's goal was to predict the outcome of atomic experiments, a goal that had eluded classical physics. The mathematical equation that he developed is now called the **Schrödinger equation.** It is the law of quantum mechanics in the same way that Newton's laws are the laws of classical mechanics. It would make sense to call it Schrödinger's law, but by tradition it is called simply the Schrödinger equation.

You learned in Chapter 40 that a matter particle is characterized in quantum physics by its wave function $\psi(x)$. If you know a particle's wave function, you can predict the probability of detecting it in some region of space. That's all well and good, but Chapter 40 didn't provide any method for determining wave functions. The Schrödinger equation is the missing piece of the puzzle. It is an equation for finding a particle's wave function $\psi(x)$ along the x-axis.

Consider an atomic particle with mass m and mechanical energy E whose interactions with the environment can be characterized by a one-dimensional potential-energy function $U(x)$. The Schrödinger equation for the particle's wave function is

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}[E - U(x)]\psi(x) \quad \text{(the Schrödinger equation)} \qquad (41.1)$$

This is a differential equation whose solution is the wave function $\psi(x)$ that we seek. Our first goal is to learn what this equation means and how it is used.

Erwin Schrödinger.

Justifying the Schrödinger Equation

The Schrödinger equation can be neither derived nor proved. It is not an outgrowth of any previous theory. Its success depended on its ability to explain the various phenomena that had refused to yield to a classical-physics analysis and to make new predictions that were subsequently verified.

Although the Schrödinger equation cannot be derived, the reasoning behind it can at least be made *plausible.* De Broglie had postulated a wave-like nature for matter in which a particle of mass m, velocity v, and momentum $p = mv$ has a wavelength

$$\lambda = \frac{h}{p} = \frac{h}{mv} \qquad (41.2)$$

Schrödinger's goal was to find a *wave equation* for which the solution would be a wave function having the de Broglie wavelength.

An oscillatory wave-like function with wavelength λ is

$$\psi(x) = \psi_0 \sin\left(\frac{2\pi x}{\lambda}\right) \qquad (41.3)$$

where ψ_0 is the amplitude of the wave function. Suppose we take a second derivative of $\psi(x)$:

$$\frac{d^2\psi}{dx^2} = \frac{d}{dx}\frac{d\psi}{dx} = -\frac{(2\pi)^2}{\lambda^2}\psi_0 \sin\left(\frac{2\pi x}{\lambda}\right)$$

We can use the definition of $\psi(x)$, from Equation 41.3, to write the second derivative as

$$\frac{d^2\psi}{dx^2} = -\frac{(2\pi)^2}{\lambda^2}\psi(x) \qquad (41.4)$$

Equation 41.4 relates the wavelength λ to a combination of the wave function $\psi(x)$ and its second derivative.

NOTE ▶ These manipulations are not specific to quantum mechanics. Equation 41.4, which is well known for classical waves, applies equally well to sound waves and waves on a string. ◀

Schrödinger's insight was to identify λ with the de Broglie wavelength of a particle. We can write the de Broglie wavelength in terms of the particle's kinetic energy K as

$$\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2m(\frac{1}{2}mv^2)}} = \frac{h}{\sqrt{2mK}} \qquad (41.5)$$

Notice that **the de Broglie wavelength increases as the particle's kinetic energy decreases.** This observation will play a key role.

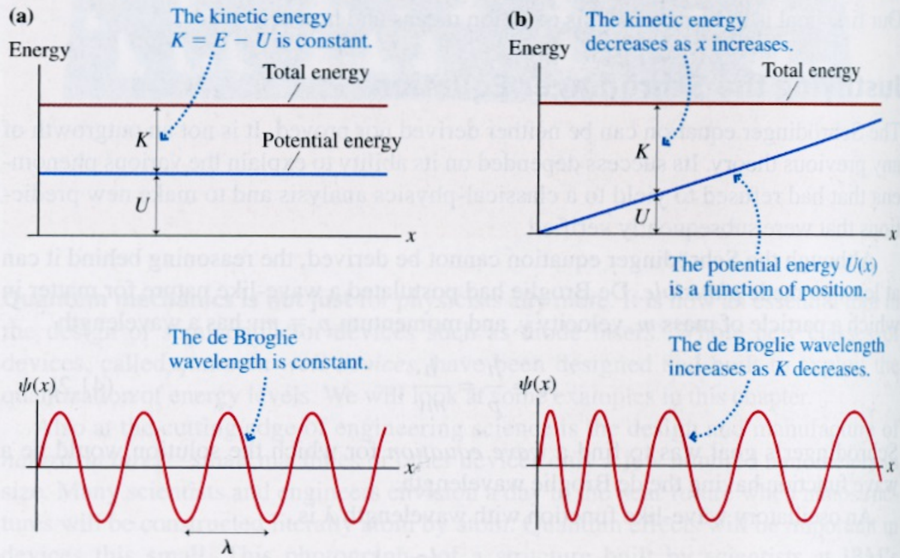
If we square this expression for λ and substitute it into Equation 41.4, we find

$$\frac{d^2\psi}{dx^2} = -\frac{(2\pi)^2 2mK}{h^2}\psi(x) = -\frac{2m}{\hbar^2}K\psi(x) \qquad (41.6)$$

where $\hbar = h/2\pi$. Equation 41.6 is a differential equation for the function $\psi(x)$. The solution to this equation is the sinusoidal wave function of Equation 41.3, where λ is the de Broglie wavelength for a particle with kinetic energy K.

Our derivation of Equation 41.6 assumed that the particle's kinetic energy K is constant. The energy diagram of **FIGURE 41.1a** reminds you that a particle's kinetic energy remains constant as it moves along the x-axis only if its potential energy U is constant. In this case, the de Broglie wavelength is the same at all positions.

FIGURE 41.1 The de Broglie wavelength changes as a particle's kinetic energy changes.



In contrast, **FIGURE 41.1b** shows the energy diagram for a particle whose kinetic energy is *not* constant. This particle speeds up or slows down as it moves along the x-axis, transforming potential energy to kinetic energy or vice versa. Consequently, its de Broglie wavelength changes with position.

Suppose a particle's potential energy—gravitational or electric or any other kind of potential energy—is described by the function $U(x)$ or $U(y)$. That is, the potential energy is a *function of position* along the axis of motion. For example, the gravitational potential energy near the earth's surface is the function $U(y) = mgy$.

If E is the particle's total mechanical energy, its kinetic energy at position x is

$$K = E - U(x) \qquad (41.7)$$

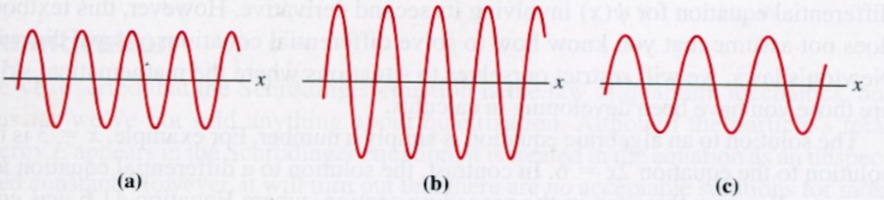
If we use this expression for K in Equation 41.6, that equation becomes

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}[E - U(x)]\psi(x)$$

This is Equation 41.1, the Schrödinger equation for the particle's wave function $\psi(x)$.

NOTE ▶ This has not been a derivation of the Schrödinger equation. We've made a *plausibility argument,* based on de Broglie's hypothesis about matter waves, but only experimental evidence will show if this equation has merit. ◀

STOP TO THINK 41.1 Three de Broglie waves are shown for particles of equal mass. Rank in order, from fastest to slowest, the speeds of particles a, b, and c.



Quantum-Mechanical Models

Long ago, in your study of Newtonian mechanics, you learned the importance of *models*. To understand the motion of an object, we made simplifying assumptions: that the object could be represented by a particle, that friction could be described in a simple way, that air resistance could be neglected, and so on. Models allowed us to understand the primary features of an object's motion without getting lost in the details.

The same holds true in quantum mechanics. The exact description of a microscopic atom or a solid is extremely complicated. Our only hope for using quantum mechanics effectively is to make a number of simplifying assumptions—that is, to make a **quantum-mechanical model** of the situation. Much of this chapter will be about building and using quantum-mechanical models.

The test of a model's success is its agreement with experimental measurement. Laboratory experiments cannot measure $\psi(x)$, and they rarely make direct measurements of probabilities. Thus it will be important to tie our models to measurable quantities such as wavelengths, charges, currents, times, and temperatures.

There's one very important difference between models in classical mechanics and quantum mechanics. Classical models are described in terms of *forces*, and Newton's laws are a connection between force and motion. The Schrödinger equation for the wave function is written in terms of *energies*. Consequently, quantum-mechanical modeling involves finding a potential-energy function $U(x)$ that describes a particle's interactions with its environment.

FIGURE 41.2 reminds you how to interpret an energy diagram. We will use energy diagrams extensively in this and the remaining chapters to portray quantum-mechanical models. A review of Section 10.7, where energy diagrams were introduced, is highly recommended. ActivPhysics ONLINE 20.1

FIGURE 41.2 Interpreting an energy diagram.