

examples of the use of Schrödinger's equation

In this chapter several examples will be presented to illustrate the use of the Schrödinger equation and the application of boundary conditions. In the process of studying these examples, the physical meaning of the wavefunction should become clearer. For simplicity, all the examples will be done only in one dimension.

1 FREE-PARTICLE GAUSSIAN WAVE PACKET

In Chapter 6 we saw that the nonrelativistic time-dependent Schrödinger equation for free particles moving in one dimension is:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = i\hbar \frac{\partial \psi}{\partial t} \quad (7.1)$$

and that a typical solution is a wavefunction of the form

$$\psi = A e^{i(px - Et)/\hbar} \quad (7.2)$$

where $E = E(p) = p^2/2m$ is the nonrelativistic kinetic energy. Physically, this solution might correspond to a beam of particles uniformly distributed along the x axis, moving with definite particle velocity, $v = p/m$, and with definite energy $E = E(p)$. The solution in Equation (7.2) is thus both a momentum eigenfunction and an energy eigenfunction.

By superposition of such eigenfunctions corresponding to different values of momentum (and energy), we can build up interesting solutions of the free-particle Schrödinger equation. For example, as was also discussed in Chapter 6, the wavefunction

$$\psi = A_1 \exp\left[\frac{i(p_1 x - p_1^2 t/2m)}{\hbar}\right] + A_2 \exp\left[\frac{i(p_2 x - p_2^2 t/2m)}{\hbar}\right] \quad (7.3)$$

with $p_1 \neq p_2$, is likewise a solution to Equation (7.2), but it is no longer a momentum or energy eigenfunction.

We now wish to discuss the quantum-mechanical description of a free particle, which corresponds more closely to our intuitive notion of a particle as being well localized in space. The solution in Equation (7.2) is certainly not well localized, because there is no information at all in this wavefunction about the x coordinate of the particle; all x coordinates are equally probable. A wavefunction describing a localized particle, with some small uncertainty Δx in position, must have a large uncertainty in momentum according to the uncertainty principle, $\Delta x \Delta p_x \geq \frac{1}{2} \hbar$. To obtain a localized wave packet, we will consider a more general superposition of free-particle momentum eigenfunctions of many different momenta. This superposition has the form:

$$\psi(x, t) = \sum_i A_i \exp\left[\frac{i(p_i x - p_i^2 t/2m)}{\hbar}\right] \quad (7.4)$$

where the numbers A_i are any constant coefficients. Since each term in Equation (7.4) satisfies the Schrödinger equation, which is a linear differential equation, the sum satisfies it.

We can also consider the superposition of wavefunctions with a continuous distribution of momenta by passing from the summation in Equation (7.4) to an integration:

$$\psi(x, t) = \int_{-\infty}^{\infty} dp A(p) \exp\left[\frac{i(px - ip^2 t/2m)}{\hbar}\right] \quad (7.5)$$

where $A(p)$ is any function of p .

Now to obtain a function which is localized in space, we shall consider the superposition in Equation (7.5), with $A(p)$ chosen to give a distribution of momenta about some central value, p_0 . If the momenta appearing in the integral in Equation (7.5) are distributed symmetrically about the value p_0 , we would expect the particle to move with an average momentum $p_0 = mv_0$. Furthermore, if there is a large spread in momenta, i.e. if Δp is large, we would expect it to be possible to have Δx small. We shall choose a distribution of momenta given by a *gaussian*, as follows:

$$A(p) = \sqrt{\frac{\sigma}{2\pi\sqrt{\pi}\hbar^2}} \exp\left[\frac{-\frac{1}{2}\sigma^2(p - p_0)^2}{\hbar^2}\right] \quad (7.6)$$

While this is only one of an infinite number of choices, the choice in Equation (7.6) is particularly interesting for several reasons and is not too difficult to handle mathematically. The constants in front of the exponential in Equation (7.6) make the function $\psi(x, t)$ a normalized one, so that the total probability is unity. Thus, we shall study the *wave packet*:

$$\psi(x, t) = \sqrt{\frac{\sigma}{2\pi\sqrt{\pi}\hbar^2}} \int_{-\infty}^{\infty} \exp\left[\frac{-\frac{1}{2}\sigma^2(p - p_0)^2}{\hbar^2}\right] \exp\left[\frac{i(px - p^2 t/2m)}{\hbar}\right] dp \quad (7.7)$$

2 PACKET AT $t = 0$

Consider first the resulting description of the particle at time $t = 0$:

$$\psi(x, t = 0) = \sqrt{\frac{\sigma}{2\pi\sqrt{\pi}\hbar^2}} \int_{-\infty}^{\infty} \exp\left[-\frac{1}{2}\frac{\sigma^2(p - p_0)^2}{\hbar^2}\right] \exp\left(\frac{ipx}{\hbar}\right) dp \quad (7.8)$$

The integral may be performed with the help of Table 7.1, after changing $e^{ipx/\hbar}$ to $e^{ip_0x/\hbar} e^{i(p-p_0)x/\hbar}$ and introducing a new integration variable by the substitution $y = p - p_0$:

$$\psi(x, t = 0) = \frac{1}{\sqrt{\sqrt{\pi}\sigma}} \exp\left(\frac{-x^2}{2\sigma^2}\right) \exp\left(\frac{ip_0x}{\hbar}\right) \quad (7.9)$$

Clearly, at this time the wavefunction is localized in space, near the origin at $x = 0$. The probability density is

$$|\psi|^2 = \frac{1}{\sqrt{\pi}\sigma} \exp\left(\frac{-x^2}{\sigma^2}\right) \quad (7.10)$$

which is a normalized gaussian distribution centered at $x = 0$. Thus at $t = 0$, $\langle x \rangle = 0$. To calculate Δx at this time, we need

$$\begin{aligned} \Delta x &= \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \left[\int_{-\infty}^{\infty} dx x^2 |\psi|^2 \right]^{1/2} \\ &= \left[\int_{-\infty}^{\infty} dx x^2 \frac{1}{\sqrt{\pi}\sigma} \exp\left(-\frac{x^2}{\sigma^2}\right) \right]^{1/2} = \frac{\sigma}{\sqrt{2}} \quad (7.11) \end{aligned}$$

from Table 7.1. Thus, σ is a measure of the distance within which the particle is initially localized.

TABLE 7.1 Some Integrals Involving Complex Exponentials

$$\int_{-\infty}^{\infty} \exp\left(-\frac{y^2}{a^2} + iby\right) dy = \sqrt{\pi} a \exp\left[-\left(\frac{ab}{2}\right)^2\right], \quad \text{Real part of } a^2 > 0$$

$$\int_{-\infty}^{\infty} \exp\left(-\frac{y^2}{a^2}\right) y^2 dy = \frac{1}{2} a^3 \sqrt{\pi}$$

$$\int_{-\infty}^{\infty} y \exp\left(-\frac{y^2}{a^2}\right) dy = 0$$

The oscillating factor $\exp(ip_0x/\hbar)$, which multiplies the gaussian in Equation (7.9), corresponds to the fact that the particle has an overall momentum p_0 ,

because, calculating the expectation value of momentum, we have:

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^* \frac{\hbar}{i} \frac{\partial \psi}{\partial x} dx = \frac{1}{\sqrt{\pi}\sigma} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{\sigma^2}\right) \left(-\frac{\hbar}{i} \frac{x}{\sigma^2} + p_0\right) dx = p_0 \quad (7.12)$$

Thus the wavefunction corresponds to a particle with average velocity, $v_0 = p_0/m$. The rms deviation from the mean momentum, or uncertainty in momentum, is:

$$\begin{aligned} \Delta p &= \left[\int_{-\infty}^{\infty} \psi^* \left(-\hbar^2 \frac{\partial^2 \psi}{\partial x^2}\right) dx - p_0^2 \right]^{1/2} \\ &= \left\{ \int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi}\sigma} \exp\left(-\frac{x^2}{\sigma^2}\right) \left[-\frac{\hbar^2 x^2}{\sigma^4} + 2i \frac{\hbar x p_0}{\sigma^2} + p_0^2 + \frac{\hbar^2}{\sigma^2} \right] dx - p_0^2 \right\}^{1/2} \\ &= \left[-\frac{1}{2} \frac{\hbar^2}{\sigma^2} + 0 + p_0^2 + \frac{\hbar^2}{\sigma^2} - p_0^2 \right]^{1/2} = \frac{\hbar}{\sqrt{2}\sigma} \quad (7.13) \end{aligned}$$

Note that at $t = 0$ the uncertainty product is the minimum allowed by the uncertainty principle,

$$\Delta p \Delta x = \frac{\hbar}{\sqrt{2}\sigma} \cdot \frac{\sigma}{\sqrt{2}} = \frac{\hbar}{2} \quad (7.14)$$

Thus, at first the gaussian wave packet is actually a minimum uncertainty packet; this is one of the reasons the gaussian packet is of particular interest.

Summarizing our results so far, we have, at $t = 0$,

$$\langle x \rangle = 0, \quad \Delta x = \frac{\sigma}{\sqrt{2}} \quad (7.15)$$

$$\langle p \rangle = p_0, \quad \Delta p = \frac{\hbar}{\sqrt{2}\sigma} \quad (7.16)$$

7.3 PACKET FOR $t > 0$

Next, we shall calculate the expectation values and uncertainties at any later time t . We would expect that the average momentum and uncertainty in momentum would not change with time, since there are no forces to modify the momentum distribution. This could be verified by detailed calculation using the ψ in Equation (7.18) below. To calculate x and Δx , we need the wavefunction $\psi(x, t)$ at an arbitrary time and hence must perform the p integral in Equation (7.7) at an arbitrary time. This may be done in a straightforward way, using the integrals in Table 7.1, although the algebra is a little messy. The integral may be written as:

$$\psi(x, t) = \sqrt{\frac{\sigma}{2\pi\sqrt{\pi}\hbar^2}} \exp\left[\frac{i(p_0x - p_0^2t/2m)}{\hbar}\right] \times \int dp \exp\left[-(p - p_0)^2\left(\frac{\sigma^2}{2\hbar^2} + \frac{it}{2m\hbar}\right) + i(p - p_0)\left(\frac{x}{\hbar} - \frac{p_0t}{m\hbar}\right)\right] \quad (7.17)$$

The first integral in Table 7.1 then gives us:

$$\psi(x, t) = \sqrt{\frac{\sigma}{\sqrt{\pi}(\sigma^2 + i\hbar t/m)}} \exp\left[\frac{1}{2}\frac{(x - p_0t/m)^2}{\sigma^2 + i\hbar t/m} + \frac{i}{\hbar}\frac{(p_0x - p_0^2t)}{2m}\right] \quad (7.18)$$

This wave function leads to a probability density of

$$\psi^*\psi = |\psi|^2 = \frac{\sigma}{\sqrt{\pi}\sqrt{\sigma^4 + \hbar^2t^2/m^2}} \exp\left[\frac{-\sigma^2(x - p_0t/m)^2}{(\sigma^4 + \hbar^2t^2/m^2)}\right] \quad (7.19)$$

This distribution is centered about the point $x = p_0t/m$, corresponding to an average particle speed of p_0/m . This agrees with the result $\langle p \rangle$ of Equation (7.12). The distribution center, p_0t/m , is, of course, also the expectation value of x . The rms deviation of x from its mean is:

$$\begin{aligned} \Delta x &= \sqrt{\left\langle \left(x - \frac{p_0t}{m}\right)^2 \right\rangle} \\ &= \left\{ \int_{-\infty}^{\infty} \frac{\sigma}{\sqrt{\pi}\sqrt{\sigma^4 + \hbar^2t^2/m^2}} \left(x - \frac{p_0t}{m}\right)^2 \exp\left[\frac{-\sigma^2(x - p_0t/m)^2}{(\sigma^4 + \hbar^2t^2/m^2)}\right] dx \right\}^{1/2} \\ &= \frac{\sqrt{\sigma^2 + \hbar^2t^2/m^2\sigma^2}}{\sqrt{2}} \quad (7.20) \end{aligned}$$

This Δx is least at $t = 0$ and increases thereafter. This is because of the possible presence of momenta greatly different from p_0 within the momentum distribution, resulting in the possibility that the particle may be moving with velocities greater or less than the average, p_0/m , and thus the possibility of the particle being farther and farther from $\langle x \rangle$ as time progresses. If the particle is very sharply localized in space initially, that is if σ is very small, then from Equation (7.20) it is seen that the wave packet will spread very rapidly, because at large times, $\Delta x \sim \hbar t/m\sigma$. This is due to the complementary presence of very high momenta, which must be present in order that Δp be large, $\Delta p \geq \hbar/2\Delta x$. If the particle is not very well localized initially, (large σ), the wave packet spreads slowly. We could expect that at sufficiently large times, the spread of the packet would be on the order of $\Delta vt = \Delta pt/m = \hbar t/2\sigma m$. The uncertainty Δx in Equation (7.20) is of this order of magnitude for large t . The uncertainty principle is satisfied at all times, since from Equations (7.12) and (7.20)

$$\Delta p \Delta x = \frac{1}{2} \hbar \sqrt{1 + \frac{\hbar^2 t^2}{m^2 \sigma^2}} \geq \frac{1}{2} \hbar \quad (7.21)$$

Let us put some numbers in, to see how long we can expect a particle to remain reasonably well localized. Suppose we consider an electron with mass of about 10^{-30} kg. If it has a few electron volts kinetic energy, such as it might pick up in a low voltage vacuum tube, it is moving with a speed of around 10^6 m/sec. Also, if in an experiment the electron is initially localized to within a distance Δx of 0.01 cm, then the spread in velocities, $\Delta v = \Delta p/m = \hbar/(2\Delta x m)$, is on the order of 1 m/sec, very small compared to the speed. Now, from Equation (7.20) the spread in the distribution will be multiplied by $\sqrt{2}$ when $\hbar t/m = \sigma^2$. Since σ is of the order of 0.01 cm, this time is of the order of 10^{-4} sec. While this may not seem a long time, with a speed of 10^6 m/sec, the electron will have gone 10^2 meters, or about 300 feet, in that time. During this displacement, the packet will spread only about 40% in width. Thus, for most macroscopic experiments, we do not have to worry about the electrons' becoming nonlocalized. For a macroscopic object, such as a stone of 100 gm mass, the time required for Δx to increase by a factor of $\sqrt{2}$ is around 10^{25} sec, or about 10^{18} years. This indicates why quantum mechanics is ordinarily unimportant for the description of macroscopic bodies. The spreading and motion of a gaussian wave packet is illustrated in Figure 7.1.

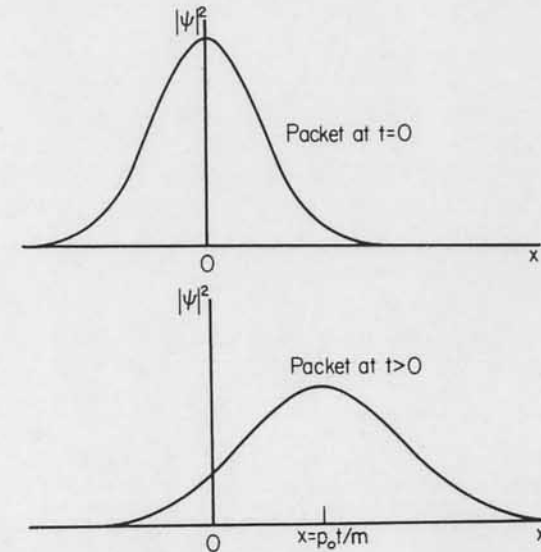


Figure 7.1. Graph of probability density in a Gaussian wave packet. The wave packet spreads in space as time progresses.

7.4 STEP POTENTIAL; HIGH ENERGY $E > V_0$

The first example involving the matching of boundary conditions will involve the one dimensional potential energy shown in Figure 7.2. This is called a *step potential*, and corresponds to the particle experiencing a very large force over a very small distance when going from region I to region II. In region I the potential energy is zero, and in region II it is the constant V_0 .