

Chapter 3

Free-Particle Schrödinger Equation: Wave Packets

The Schrödinger equation is the fundamental equation of non-relativistic quantum mechanics. As with any equation in physics, its validity relies on experimental verification of the predictions of the equation. So far, it appears that there are no experiments that are inconsistent with quantum mechanics. As you shall see, it is not always easy to test the predictions of the Schrödinger equation. In other words, mapping out the probability distribution associated with a quantum system can represent a formidable task. Moreover, quantum mechanics is far from a complete theory since it does not address the dynamic evolution of the wave function when a measurement is made. Nevertheless, the success of the Schrödinger equation in describing the wave nature of matter and the energy level structure of atoms, molecules, and solids is beyond question.

In this chapter, I discuss the Schrödinger equation for a free particle, a particle not subjected to forces. Even though I use the word “particle” throughout this book, it is a misnomer in many cases since the particle is actually acting as a wave. It is not possible to *derive* Schrödinger’s equation; it is essentially a postulate of quantum mechanics. However, it is possible to use an analogy with the wave equation of electromagnetism, plus some additional ingredients, to cook up an equation that turns out to be the time-dependent Schrödinger equation for a free particle. This is the recipe I shall follow.

I want to remind you of an admonition given in Chap. 1. The following chapters contain many mathematical expressions. Rather than focus on the mathematical details, you should always try to have a general idea of where the calculations are going. In other words, what physical features of a specific problem are being analyzed? Try not to let the mathematics obscure the underlying physical processes under investigation.

3.1 Electromagnetic Wave Equation: Pulses

Maxwell's equations imply that both the electric and magnetic fields obey wave equations. The wave equation for the electric field vector $\mathbf{E}(\mathbf{R}, t)$ of light in vacuum is

$$\nabla^2 \mathbf{E}(\mathbf{R}, t) = \frac{1}{c^2} \frac{\partial^2 \mathbf{E}(\mathbf{R}, t)}{\partial t^2}, \quad (3.1)$$

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (3.2)$$

is defined here in terms of its rectangular components and c is the speed of light. A solution of this equation that also satisfies Maxwell's equations for the electric field is

$$\mathbf{E}(\mathbf{r}, t) = \hat{\mathbf{e}} E e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} + \text{c.c.}, \quad (3.3)$$

provided

$$\omega = kc \quad (3.4)$$

and

$$\mathbf{k} \cdot \hat{\mathbf{e}} = 0, \quad (3.5)$$

where $\hat{\mathbf{e}}$ is a unit polarization vector for the field. Equation (3.5) must be satisfied to insure that $\nabla \cdot \mathbf{E}(\mathbf{r}, t) = 0$. There are two independent polarizations for each field frequency and the direction of polarization is perpendicular to the propagation vector \mathbf{k} of the field (the field is *transverse*). The abbreviation c.c. in Eq. (3.3) stands for *complex conjugate*.

The field in Eq. (3.3) corresponds to an infinite, monochromatic, plane wave and is a basic building block solution of Maxwell's wave equation. It is possible to construct *any* field pulse using a superposition of such states. To simplify matters, I consider only one polarization component of the field and a plane wave field. For an arbitrary plane wave field propagating in the *positive* x direction and polarized in the z direction, the electric field can be written as

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{u}_z E(x, t), \quad (3.6)$$

where \mathbf{u}_z is a unit vector in the z direction and the amplitude $E(x, t)$ can be expanded as

$$E(x, t) = \frac{1}{\sqrt{2\pi}} \int_0^\infty dk A(k) e^{i(kx - \omega t)} + \text{c.c.} \quad (3.7)$$

The integral over k has been restricted to positive values to ensure that each component of the wave propagates in the positive x direction. It is a simple matter to show that Eq. (3.6) with $E(x, t)$ given by Eq. (3.7) is also a solution of the wave equation, provided $\omega = kc > 0$. Moreover, since $\omega = kc$,

$$E(x, t) = \frac{1}{\sqrt{2\pi}} \int_0^\infty dk A(k) e^{ik(x-ct)} + \text{c.c.} = E(x - ct, 0). \quad (3.8)$$

The pulse amplitude is simply the original pulse amplitude translated by ct ; in other words, the pulse propagates *without distortion* at a speed equal to the speed of light.

3.2 Schrödinger's Equation

I want to use Einstein's concept of photons and de Broglie's concept of matter waves to make a plausible transition from the wave equation of electromagnetism to the Schrödinger equation of quantum mechanics. I start by using Einstein's expression for the energy E (not to be confused with the field amplitude) associated with "photons" having frequency $f = \omega/2\pi$,

$$E = hf = \hbar\omega, \quad (3.9)$$

to transform Eq. (3.8) into

$$E(x, t) = \frac{1}{\sqrt{2\pi}} \int_0^\infty dk A(k) e^{i(kx - Et/\hbar)} + \text{c.c.} \quad (3.10)$$

I now look for a wave function for *matter waves* having a similar form, namely

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty dk \Phi(k) e^{i(kx - Et/\hbar)}. \quad (3.11)$$

Although the electric field amplitude $E(x, t)$ is real, it is assumed that the *wave function* $\psi(x, t)$ can be complex. The final step of the "derivation" is to use de Broglie's relation

$$p = \hbar k, \quad (3.12)$$

to write the energy E for a free particle having mass m in terms of k as

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}. \quad (3.13)$$

With this assignment, Eq. (3.11) becomes

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty dk \Phi(k) \exp[i(kx - \hbar k^2 t/2m)]. \quad (3.14)$$

It is not difficult to prove that $\psi(x, t)$ satisfies the partial differential equation

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2}, \quad (3.15)$$

which can be generalized to three dimensions as

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, t). \quad (3.16)$$

Equation (3.16) is recognized as the time-dependent Schrödinger equation for a free particle. Of course, some physical interpretation must be given to $\psi(\mathbf{r}, t)$. As an additional postulate, I assume that $|\psi(\mathbf{r}, t)|^2$ is the probability density to find the particle at position \mathbf{r} at time t .

Equation (3.14) differs from Eq. (3.7) in a fundamental way since the dispersion relation (relation between ω and k) in Eq. (3.14) is not linear,

$$\omega = \frac{E}{\hbar} = \frac{\hbar k^2}{2m}. \quad (3.17)$$

As a result, waves having different values of k or p propagate at different velocities. Since the matter wave pulse, referred to as a *wave packet*, has components that propagate with different velocities and since no forces act on the particle, the shape of the wave packet changes in time, unlike that for a plane wave optical field pulse in vacuum.

3.2.1 Wave Packets

Now that I have defined the wave function, I can try to construct something that looks like a “particle.” The term “particle” can be somewhat confusing. First of all, I am considering a wave theory, so I have to define what I mean by a “particle.” Moreover, particles in classical physics necessarily have some internal structure and finite spatial extent. For the most part, the particles to which I refer in quantum mechanics correspond to idealized *point particles* in classical physics.

Let me start from the wave function in three dimensions for a matter wave corresponding to a point particle having mass m , that is, a generalization of Eq. (3.14) to three dimensions. It is not difficult to show that the wave function

$$\psi(\mathbf{r}, t) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{k} \Phi(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{r} - \hbar k^2 t/2m)}. \quad (3.18)$$

is a solution of time-dependent Schrödinger equation in three dimensions, Eq. (3.16). To model a particle, the momentum, or equivalently, the propagation

vector \mathbf{k} (since $\mathbf{k} = \mathbf{p}/\hbar$) must be fairly well defined. In other words, I must choose $|\Phi(\mathbf{k})|^2$ to be non-vanishing only for those values of \mathbf{k} satisfying $|\mathbf{k} - \mathbf{k}_0| \lesssim k_0$, where $\mathbf{k}_0 = \bar{\mathbf{k}}$ and Δk is the standard deviation of k for the distribution $|\Phi(\mathbf{k})|^2$. Moreover, if $|\Phi(\mathbf{k})|^2$ is meant to represent a particle, it should be a smooth function having a maximum at $\mathbf{k} = \mathbf{k}_0$ that falls monotonically to zero in all directions (in k space) for $|\mathbf{k} - \mathbf{k}_0| > \Delta k$. In other words, $|\Phi(\mathbf{k})|^2$ is a sharply peaked function centered at $\mathbf{k} = \mathbf{k}_0$ having width of order Δk . I need to approximate the exponential function appearing in Eq. (3.18) when $\mathbf{k} \approx \mathbf{k}_0$.

It helps to write

$$\begin{aligned}\mathbf{k} &= \mathbf{k}_0 + (\mathbf{k} - \mathbf{k}_0), \\ k^2 &= [\mathbf{k}_0 + (\mathbf{k} - \mathbf{k}_0)]^2 = -k_0^2 + 2\mathbf{k}_0 \cdot \mathbf{k} + |\mathbf{k} - \mathbf{k}_0|^2,\end{aligned}\quad (3.19)$$

allowing me to transform Eq. (3.18) into

$$\begin{aligned}\psi(\mathbf{r}, t) &= \frac{e^{i\hbar k_0^2 t/2m}}{(2\pi)^{3/2}} \int_{-\infty}^{\infty} d\mathbf{k} \Phi(\mathbf{k}) \\ &\times \exp\left\{i\left[\mathbf{k} \cdot (\mathbf{r} - \hbar\mathbf{k}_0 t/m) - \hbar|\mathbf{k} - \mathbf{k}_0|^2 t/2m\right]\right\}.\end{aligned}\quad (3.20)$$

For the moment, suppose that I can neglect the $\hbar|\mathbf{k} - \mathbf{k}_0|^2 t/2m$ term in the exponent,

$$\hbar|\mathbf{k} - \mathbf{k}_0|^2 t/2m \ll 1. \quad (3.21)$$

Then, for all values of \mathbf{k} that contribute significantly to the integral,

$$\begin{aligned}\psi(\mathbf{r}, t) &\approx \frac{e^{i\hbar k_0^2 t/2m}}{(2\pi)^{3/2}} \int_{-\infty}^{\infty} d\mathbf{k} \Phi(\mathbf{k}) e^{i\mathbf{k} \cdot (\mathbf{r} - \hbar\mathbf{k}_0 t/m)} \\ &= e^{i\hbar k_0^2 t/2m} \psi(\mathbf{r} - \mathbf{v}_0 t, 0),\end{aligned}\quad (3.22)$$

where

$$\mathbf{v}_0 = \frac{\hbar\mathbf{k}_0}{m} = \frac{\mathbf{p}_0}{m} \quad (3.23)$$

is the average velocity of the particle.

Aside from a phase factor, $\psi(\mathbf{r}, t)$ propagates as an undistorted wave having momentum \mathbf{p}_0 . If the initial distribution $|\psi(\mathbf{r}, 0)|^2$ is non-vanishing only in a small volume centered at $\mathbf{r} = \mathbf{0}$, then the distribution $|\psi(\mathbf{r}, t)|^2$ will be non-vanishing only in a small volume centered at $\mathbf{r} = \mathbf{v}_0 t$; in other words, the distribution function can mirror the behavior of “particle” that is moving with velocity \mathbf{v}_0 . How localized can the particle be? When can condition (3.21) be satisfied? It certainly fails if I let

t get arbitrarily large. Many of these questions can be answered by considering a specific wave function and seeing how it propagates. I will calculate $|\psi(x, t)|^2$ for a one-dimensional Gaussian wave packet that is centered at $x = 0$ at $t = 0$.

3.2.1.1 Gaussian Wave Packet

At $t = 0$, I take the wave function for a particle having mass m to be

$$\psi(x, 0) = \frac{1}{(\pi\sigma^2)^{1/4}} e^{-x^2/2\sigma^2} e^{ik_0x}, \quad (3.24)$$

such that

$$|\psi(x, 0)|^2 = \frac{1}{(\pi\sigma^2)^{1/2}} e^{-x^2/\sigma^2} \quad (3.25)$$

is a Gaussian centered at the origin with a full-width at half maximum (FWHM) equal to 1.67σ . The normalization has been chosen such that

$$\int_{-\infty}^{\infty} dx |\psi(x, 0)|^2 = 1. \quad (3.26)$$

I want to find $\psi(x, t)$. To do so, I must first find $\Phi(k)$ and then use Eq. (3.14) to get $\psi(x, t)$. The factor of e^{ik_0x} in Eq. (3.24) leads to an average velocity for the packet equal to $\hbar k_0/m$, as you shall see.

It follows from Eq. (3.14) that

$$\psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \Phi(k) e^{ikx}. \quad (3.27)$$

I take the inverse Fourier transform of this equation to obtain

$$\begin{aligned} \Phi(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \psi(x, 0) e^{-ikx} \\ &= \frac{1}{\sqrt{2\pi}} \frac{1}{(\pi\sigma^2)^{1/4}} \int_{-\infty}^{\infty} dx e^{-x^2/2\sigma^2} e^{ik_0x} e^{-ikx}. \end{aligned} \quad (3.28)$$

The integral is tabulated or can be evaluated using contour integration. In either case, one finds

$$\Phi(k) = \left(\frac{\sigma^2}{\pi}\right)^{1/4} e^{-(k-k_0)^2\sigma^2/2}; \quad (3.29)$$

$$|\Phi(k)|^2 = \left(\frac{\sigma^2}{\pi}\right)^{1/2} e^{-(k-k_0)^2\sigma^2}. \quad (3.30)$$

The k -space distribution is *also* a Gaussian, centered at $k = k_0$, having FWHM equal to $1.67/\sigma$.

The variance of x at $t = 0$ is

$$[\Delta x(t=0)]^2 = \langle x^2(t=0) \rangle = \int_{-\infty}^{\infty} dx x^2 |\psi(x, 0)|^2 = \frac{\sigma^2}{2} \quad (3.31)$$

and the variances of k and p are

$$(\Delta k)^2 = \langle (k - k_0)^2 \rangle = \int_{-\infty}^{\infty} dk (k - k_0)^2 |\Phi(k)|^2 = \frac{1}{2\sigma^2}; \quad (3.32a)$$

$$(\Delta p)^2 = \frac{\hbar^2}{2\sigma^2}, \quad (3.32b)$$

such that

$$\Delta x(t=0)\Delta k = \frac{1}{2}; \quad (3.33a)$$

$$\Delta x(t=0)\Delta p = \frac{\hbar}{2}. \quad (3.33b)$$

As you shall see, this corresponds to what is called a *minimum-uncertainty wave packet*, having the minimum value of $\Delta x \Delta p$ allowed for solutions of Schrödinger's equation. The momentum distribution and Δp do not change in time since no forces act on the particle.

Owing to the spread of momenta in the wave packet, however, Δx *does* change as a function of time. The wave packet is no longer a minimum uncertainty packet for $t > 0$. Using Eqs. (3.14) and (3.29), I calculate

$$\begin{aligned} \psi(x, t) &= \frac{1}{\sqrt{2\pi}} \left(\frac{\sigma^2}{\pi} \right)^{1/4} \int_{-\infty}^{\infty} dk e^{-(k-k_0)^2 \sigma^2 / 2} e^{i(kx - \hbar k^2 t / 2m)} \\ &= \frac{e^{ik_0(x - \frac{v_0 t}{2})}}{\sqrt{2\pi}} \left(\frac{\sigma^2}{\pi} \right)^{1/4} \int_{-\infty}^{\infty} dk' e^{-k'^2 (\sigma^2 + i\hbar t / m) / 2} e^{ik'(x - v_0 t)}, \end{aligned} \quad (3.34)$$

where $k' = k - k_0$ and

$$v_0 = \hbar k_0 / m = p_0 / m. \quad (3.35)$$

The integral is tabulated or can be evaluated using contour integration and the result is

$$\psi(x, t) = \left(\frac{\sigma^2}{\pi} \right)^{1/4} \frac{e^{ik_0(x - \frac{v_0 t}{2})}}{[\sigma^2 + \frac{i\hbar t}{m}]^{1/2}} \exp \left(\frac{-(x - v_0 t)^2}{2[\sigma^2 + \frac{i\hbar t}{m}]} \right). \quad (3.36)$$

As a consequence,

$$|\psi(x, t)|^2 = \left(\frac{1}{\pi\sigma(t)^2} \right)^{1/2} e^{-(x-v_0t)^2/\sigma(t)^2}, \quad (3.37)$$

with

$$\sigma(t)^2 = \sigma^2 + \left(\frac{\hbar t}{m\sigma} \right)^2. \quad (3.38)$$

The FWHM at any time is $1.67\sigma(t)$ and $\Delta x(t) = \sigma(t)/\sqrt{2}$, such that

$$\Delta x(t)\Delta p = \frac{\hbar\sigma(t)}{2\sigma} = \frac{\hbar}{2} \left[1 + \left(\frac{\hbar t}{m\sigma^2} \right)^2 \right]^{1/2} \geq \frac{\hbar}{2}. \quad (3.39)$$

The packet remains Gaussian but spreads owing to the spread of momenta in the original packet. To see how $\Delta x(t)$ depends on Δp , I use the relationships $\Delta x(0) = \sigma/\sqrt{2}$ and $\Delta v = \Delta p/m = \hbar/(\sqrt{2}m\sigma)$ to rewrite $\Delta x(t)^2$ as

$$\begin{aligned} \Delta x(t)^2 &= \frac{\sigma(t)^2}{2} = \frac{\sigma^2}{2} + \frac{1}{2} \left(\frac{\hbar t}{m\sigma} \right)^2 \\ &= \Delta x(0)^2 + (\Delta v)^2 t^2. \end{aligned} \quad (3.40)$$

Although I have chosen a Gaussian wave packet, Eq. (3.40) turns out to be *exact* for any square-integrable initial wave function of the form $\psi(x, 0) = f(x)e^{ik_0x}$, for real $f(x)$ (see Problem 5.14–15 in Chap. 5). The variance of the wave packet is its *initial* variance plus a contribution attributable to the variance of the velocity components contained in the packet. For sufficiently large times, $\Delta x(t) \sim \Delta vt$.

I am now in a position to see when the wave packet can correspond to a classical particle. Free particles have never heard about wave packets; wave packets are a construct of physicists. For the wave packet to correspond to a particle, however, the uncertainties in position and momentum must satisfy

$$\Delta x(t) \ll x_0; \quad \Delta p \ll p_0 \quad (3.41)$$

subject to the restriction

$$\Delta x(0)\Delta p \geq \frac{\hbar}{2}. \quad (3.42)$$

The quantities x_0 and p_0 are determined by the problem. You can think of them as the smallest possible resolution in position and momentum that can be detected in a given experiment. In bound state problems they could correspond

to some typical bound state radius and magnitude of bound state momentum for the bound particle. For the free particle, let's take $x_0 = 10^{-8}$ m and $v_0 = 10^{-7}$ m/s, which locates the particle to better than an optical wavelength and fixes its velocity to about three meters per year. We might be able to accomplish this by using spatial filters (e.g., slits) to select both the position and range of velocities. For a one gram mass, suppose we take $\Delta x(0) = 10^{-11}$ m which implies that $\Delta v = \Delta p/m \approx \hbar/[m\Delta x(0)] \approx 10^{-20}$ m/s [admittedly, it would be difficult to create such a small wave packet]. This is a "classical" particle at $t = 0$ according to my definition since it obeys conditions (3.41). At what time t would the spreading be sufficient to render the particle "unclassical"? Arbitrarily, let's say the particle is no longer classical if $\Delta x(t) = x_0/100 = 10^{-10}$ m, which occurs for $t = 10^{10}$ s, 300 years! The bottom line is that spreading is unimportant as long as the de Broglie wavelength is much smaller than any characteristic length in the problem, such as the width of the initial wave packet. On the other hand, if you confine a free particle wave packet to a distance equal to its de Broglie wavelength, the spread in momentum in the wave packet is of order of the average momentum in the packet; as such spreading is important and the particle can no longer be viewed as a classical particle.

A simple example that illustrates the necessity of using a quantum description of matter can be found in an experiment related to *atom optics*. Suppose a well-collimated, pulsed atomic beam having velocity v_0 in the z direction is incident on a circular aperture having diameter d that is located in the xy plane. Moreover, assume that the de Broglie wavelength of the atoms, $\lambda_{dB} \ll d$. The atoms are treated as point particles, so another implicit assumption is that the atomic size is much smaller than d as well. After traversing the aperture at $t = 0$, you can think of the initial wave packet as a short pulse in the z direction having a cross-sectional area equal to $\pi d^2/4$. The transverse uncertainty in the momentum of this beam is of order $\Delta p_{\perp} \approx \hbar/d$. Matter wave effects become important when the transverse spreading is of order d , that is, for times t greater than some critical time t_F defined by

$$\Delta p_{\perp} t_F / m \approx \hbar t_F / (dm) \approx d, \quad (3.43)$$

where m is the mass of an atom in the beam. Since $t \approx z/v_0$ where z is the distance from the screen containing the aperture, the distance z_F corresponding to the time t_F is

$$z_F = v_0 t_F \approx \frac{mv_0 d^2}{\hbar} \approx \frac{d^2}{\lambda_{dB}}. \quad (3.44)$$

For $z \ll z_F$, the scattering of the particles by the slit is in the *shadow region* and the atomic motion can be treated classically. However for $z \gtrsim z_F$, diffraction plays an important role and a wave theory is needed. The situation is analogous to the scattering of optical radiation having wavelength λ by an aperture having diameter d . For distances $z \ll z_F = d^2/\lambda$ from the diffracting screen, a geometrical picture of light rays can be used, but once $z \gtrsim z_F$, diffraction effects become important and a wave theory of light is needed. In the optical case the region with $z \approx z_F$ corresponds to *Fresnel diffraction*.

Perhaps the best way to create a well-defined wave packet is to trap and cool an atom in the potential well of an *optical lattice*. An optical lattice is formed by using pairs of counter-propagating laser beams. These pairs of fields form standing wave patterns that can be used to trap neutral atoms owing to a spatially varying potential that is experienced by the atoms in the fields. Moreover the atoms can be cooled to the point where they are in the ground state of the potential. As such, if you trap one atom in one well, you have a pretty good idea of its wave function. If you suddenly remove the potential by turning off the fields, you have an initial condition in which the atom is in its ground state and has a center-of-mass wave function given by the ground state of the potential. You could let this wave packet propagate for some time and then restore the lattice and determine how far the packet has moved by seeing which well it is in. Although this experiment has yet to be carried out, the technology is now at the point where it is feasible.

3.2.2 Free-Particle Propagator

Instead of calculating $\Phi(k)$ from $\psi(x, 0)$ for each wave packet, it is possible to relate $\psi(x, t)$ *directly* to an integral of $\psi(x, 0)$. To do so I first calculate

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx' \psi(x', 0) e^{-ikx'} \quad (3.45)$$

and substitute the result into Eq. (3.14) to obtain

$$\psi(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx' \psi(x', 0) \int_{-\infty}^{\infty} dk \exp \{i[k(x-x') - \hbar k^2 t/2m]\}. \quad (3.46)$$

The integral over k is tabulated and I can write the final result as

$$\psi(x, t) = \int_{-\infty}^{\infty} dx' K(x-x', t) \psi(x', 0), \quad (3.47)$$

where the *free-particle propagator* $K(x-x', t)$ is given by

$$K(x-x', t) = \frac{1}{2\sqrt{\pi b i}} e^{i(x-x')^2/4b} \quad (3.48)$$

and

$$b = \hbar t/2m. \quad (3.49)$$

As an example of the use of the propagator, I consider an initial state wave function

$$\psi(x, 0) = \begin{cases} \frac{1}{\sqrt{a}} & |x| \leq a/2 \\ 0 & \text{otherwise} \end{cases}. \quad (3.50)$$

Since the probability density $|\psi(x, 0)|^2$ has sharp boundaries, we should expect these sharp boundaries to give rise to diffraction. From Eqs. (3.47) to (3.50), I calculate

$$\psi(x, t) = \frac{1}{2\sqrt{\pi abi}} \int_{-a/2}^{a/2} dx' e^{i(x-x')^2/4b}, \quad (3.51)$$

where b is given in Eq. (3.49). The limits on the integral have been set equal to $\pm a/2$ since $\psi(x', 0) = 0$ for $|x'| > a/2$. The integral is tabulated in terms of error functions, but I present the results rather than give formal expressions for $|\psi(x, t)|^2$.

It is usually best to give plots in terms of dimensionless variables. In this case, it is clear that x/a is an appropriate dimensionless coordinate. It would make sense to choose a dimensionless time as

$$\tau = \frac{\Delta v t}{a} = \frac{\Delta p}{ma} t, \quad (3.52)$$

where $\Delta p = m\Delta v$ is the momentum uncertainty. Unfortunately, $\Delta p = \infty$ for this wave packet, since the envelope of the absolute square of the Fourier transform of the packet,

$$|\Phi(p)|^2 = \frac{1}{2\pi\hbar a} \left| \int_{-a/2}^{a/2} dx e^{-ipx/\hbar} \right|^2 = \frac{a}{2\pi\hbar} \frac{\sin^2(pa/2\hbar)}{(pa/2\hbar)^2}, \quad (3.53)$$

falls off as p^{-2} for large p , resulting in $\langle p^2 \rangle = \infty$. However, the *central lobe* of $|\Phi(p)|^2$ has a HWHM of order $\delta p \equiv \hbar/\Delta x(0)$, where $\Delta x(0) = a/\sqrt{12}$ is the standard deviation of the initial wave packet in coordinate space.¹

If I set $\Delta p = \delta p \equiv \hbar/\Delta x(0) = 2\sqrt{3}\hbar/a$ in Eq. (3.52), then

$$\tau = \frac{2\sqrt{3}\hbar t}{ma^2} = \frac{4\sqrt{3}b}{a^2} \quad (3.54)$$

is an appropriate dimensionless time, and Eq. (3.51) can be written as

$$\psi(\xi, \tau) = \sqrt{\frac{\sqrt{3}}{\pi a \tau i}} \int_{-1/2}^{1/2} d\xi' e^{\sqrt{3}i(\xi-\xi')^2/\tau}, \quad (3.55)$$

with $\xi = x/a$ and $\xi' = x'/a$. The integral can be evaluated numerically or in terms of error functions. The dimensionless quantity $a|\psi(\xi, \tau)|^2$ is plotted in Fig. 3.1 for $\tau = 0, 0.25, 1$. The probability distribution $a|\psi(\xi, \tau)|^2$ evolves into a Fresnel-like diffraction pattern for $0 \lesssim \tau \lesssim 1$ and into a Fraunhofer diffraction pattern for $\tau \gtrsim 1$.

¹The calculated value of the HWHM of the central lobe is $0.81\hbar/\Delta x(0)$.

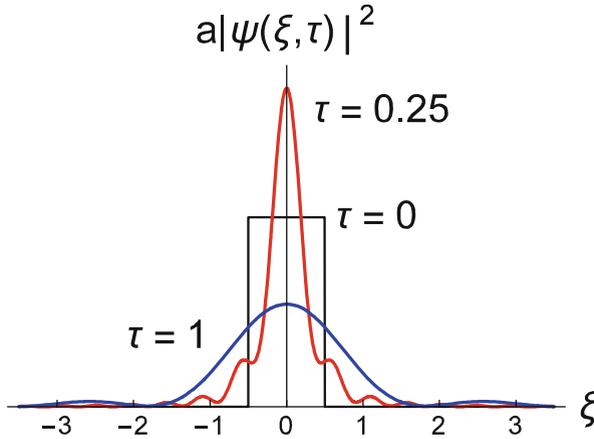


Fig. 3.1 Time evolution of the dimensionless probability distribution for a “square” wave packet. The original square packet ($\tau = 0$) undergoes Fresnel-like diffraction ($\tau = 0.25$) before assuming the Fraunhofer diffraction pattern of a single slit ($\tau = 1.0$). The dimensionless time τ is defined in Eq. (3.54)

Diffraction effects from the sharp edges of the wave packet are seen clearly in these diagrams. Although not evident from the figure, it turns out that $\Delta\xi(\tau) = \infty$ for any $\tau > 0$, since for fixed τ and $\xi \gg 1$ (see problems),

$$a|\psi(\xi, \tau)|^2 \sim \tau \frac{\sin^2\left(\sqrt{3}\xi/\tau\right)}{\sqrt{3\pi}\xi^2}. \quad (3.56)$$

This asymptotic form can be obtained by expressing the integral in Eq. (3.55) in terms of error functions and taking the asymptotic limit of the error functions. Equation (3.56) is also a good approximation to $a|\psi(\xi, \tau)|^2$ for fixed ξ and $\tau \gtrsim 1$. It represents the Fraunhofer diffraction pattern of a single slit.

The fact that $\langle \hat{p}^2 \rangle = \infty$ and $\Delta x(\tau) = \infty$ for any $\tau > 0$ is linked to sharp edges of the initial coordinate space wave packet. In fact, it is possible to show that the same features occur for any initial wave function that possesses a point jump discontinuity. In practice it is impossible to create a wave packet having a point jump discontinuity. To do so would require an infinite amount of energy since the resulting packet has $\langle p^2 \rangle = \infty$. Of course, the Schrödinger equation is a non-relativistic equation so that the momentum distribution is suspect for momenta $|p| \gtrsim mc$.

3.3 Summary

I have shown that it is possible to obtain Schrödinger's equation for a free particle, using an analogy with optical pulse propagation, along with de Broglie's definition of the wavelength of matter and Einstein's definition of the energy of a photon. The resultant free particle wave packet differs in a fundamental way from that of an optical pulse, since the dispersion relation relating energy to the momentum is quadratic for matter and linear for light. As a consequence, optical pulses in vacuum propagate without changing their shape, while free-particle, matter wave packets contain several momentum components and necessarily change their shape as a function of time.

3.4 Problems

1. Suppose that a smooth wave packet has $\Delta x(0) = a$ and $\Delta p = \alpha \hbar/a$, where $\alpha \geq 1/2$ is a constant. Explain why

$$\Delta x(t) = \sqrt{a^2 + \alpha^2 \left(\frac{\hbar t}{ma}\right)^2},$$

is not a bad guess for the width of the wave packet at any time. Using this guess with $\alpha = 1$, find the time it takes for a wave packet that is confined to its de Broglie wavelength to spread to twice its initial width in terms of the particle's energy and Planck's constant.

2. Using the result of Problem 3.1 and assuming that you are a point particle having mass 50 kg and are localized to 1.0×10^{-11} m, calculate how long it would take for you to spread by an amount equal to this initial localization distance.

3–4. Start with a one-dimensional wave packet in coordinate space. Take a wave function such as $\psi(x) = Ne^{-x^4}$ or $\psi(x) = Ne^{-x^6}$, for which no *simple* analytic solution exists for its Fourier transform. Normalize your wave function using numerical integration to find the value of N . Plot $|\psi(x)|^2$. Using Mathematica, Matlab, or Maple (or any other program you have), use numerical integration [NIntegrate in Mathematica] to obtain and plot the k -space distribution associated with the wave packet you chose. How does it differ from a Gaussian? Why? Calculate the value of $\Delta x \Delta k$ using numerical integration. In this problem, both x and k are dimensionless variables.

5. Sodium atoms moving at 1000 m/s are incident on a slit having a width of 100 nm. At 3 m from the slit, what is the approximate transverse width associated with the sodium atom's wave function? Is diffraction important in this case? These are typical values for experiments in atom optics.

6. Prove that

$$\psi(\mathbf{r}, t) = e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} e^{-ip^2t/2m\hbar}$$

is a solution of

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, t)$$

As a consequence, why is

$$\psi(\mathbf{r}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int d\mathbf{p} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} e^{-ip^2t/2m\hbar} \Phi(\mathbf{p})$$

also a solution of the equation, where $\Phi(\mathbf{p})$ is some arbitrary function for which $|\psi(\mathbf{r}, t)|^2$ is square integrable? Note that you can also write this equation as

$$\psi(\mathbf{r}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int d\mathbf{p} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \Phi(\mathbf{p}, t),$$

where

$$\Phi(\mathbf{p}, t) = e^{-ip^2t/2m\hbar} \Phi(\mathbf{p}).$$

In general it is assumed that $\psi(\mathbf{r}, t)$ and $\Phi(\mathbf{p}, t)$ are Fourier transforms of one another, even for cases when a potential is present. When a spatially varying potential is present, explain why $\Phi(\mathbf{p}, t)$ can no longer be equal to $e^{-ip^2t/2m\hbar} \Phi(\mathbf{p})$.

7–8. Return to Problem 2.3–4 for an initial (normalized) wave function

$$\psi(x, 0) = \frac{1}{2^{3/8} \sqrt{a} \sqrt{\Gamma(5/4)}} \exp(-x^4/a^4) = \frac{0.810}{\sqrt{a}} \exp(-x^4/a^4),$$

where a is a real constant and Γ is the gamma function. Calculate Δk^2 numerically and show that it is equal to $1.43/a^2$. Suppose you want to check the validity of Eq. (3.40) for this initial wave packet. Show that Eq. (3.40) can be written as

$$\Delta x^2(b) = \Delta x^2(0) + 4\Delta k^2 b^2,$$

where $b = \hbar t/2m$ and m is the mass of the particle. Evaluate $\Delta x^2(b)/a^2$ for $b/a^2 = 0, 0.1, 0.5, 0.75, 1, 5, 10$. Now use Eq. (3.47) to obtain an integral expression for $\psi(x, b)$, and numerically evaluate $\Delta x^2(b)/a^2$ for the same values of b/a^2 to see how well the equation $\Delta x^2(b) = \Delta x^2(0) + 4\Delta k^2 b^2$ agrees with the exact result. As noted in the text, the agreement should be exact in this case.

9. Use Mathematica or some other program to evaluate the integral in Eq. (3.55) in terms of error functions. Take the asymptotic limit of the result for $\xi \gg 1$ to derive Eq. (3.56) and show that $\Delta x(\tau) = \infty$ for any $\tau > 0$. Also, starting from Eq. (3.55), show that Eq. (3.56) is the correct asymptotic limit for $\tau \gg 1$ and any ξ .

10. Plot $a |\psi(\xi, \tau)|^2$ for $\psi(\xi, \tau)$ given in Eq. (3.55) as a function of ξ for $\tau = 0.001, 0.05, 0.1, 0.2$. This will show you the transition from the shadow region to that of Fresnel diffraction. Also plot $a |\psi(0, \tau)|^2$ for $0 \leq \tau \leq 0.5$ and find the maximum value it can have.

11. Assume that a wave function has the form

$$\psi(x, 0) = f(x)\Theta(a-x)\Theta(b+x),$$

where a and b are positive and $f(x)$ is a real analytic function that is non-vanishing at $x = a, b$. The Heaviside function $\Theta(x)$ is equal to 0 for $x < 0$ and 1 for $x \geq 0$, so the Heaviside functions truncate the wave function and confine it to $-b < x < a$. By evaluating the Fourier transform of $\psi(x, 0)$ for large momenta, prove that $\langle p^2 \rangle = \infty$. [Hint: an integration by parts might help.]

12. For the initial wave packet of the previous problem, use Eqs. (3.47) and (3.48) to show that $\langle x^2 \rangle = \infty$ for any $t > 0$.