Chapter 6
Problems in One-Dimension: General Considerations, Infinite Well Potential, Piecewise Constant Potentials, and Delta Function Potentials

The simplest solutions of the Schrödinger equation are those involving one-dimensional problems. Of course, nature is three dimensional, but sometimes problems can be reduced to an effective one-dimensional problem. For example, if an optical field is incident normally on a dielectric slab, the problem is essentially a one-dimensional problem. Even more important, however, is that many features of quantum mechanics are illustrated using one-dimensional problems. In this chapter, I consider some general features of solutions of the Schrödinger equation in one dimension, discuss the infinite square well potential, look at other piecewise constant potentials, and examine the one-dimensional Dirac delta function potential. In the Appendix, I discuss periodic potentials and their relation to so-called *Bloch state* wave functions. The harmonic oscillator potential in one dimension is analyzed in Chap. 7.

6.1 General Considerations

Without specifying the exact form of the potential, I can characterize the types of solutions that can exist in one dimension. That is, I can determine if there is energy degeneracy, if bound states might exist, and if the eigenvalues are continuous or discrete. For example, we know already that for a free particle in one-dimension there is a two-fold energy degeneracy and that the energy eigenvalues are continuous. The degeneracy can be understood as arising from the fact that, for the same energy, a particle can be moving to the right or left. This can be viewed as a *left-right degeneracy*. In the examples given below, I always set the zero of energy such that the potential as $|x| \to \infty$ is positive or zero. In one-dimensional problems there can never be more than a two-fold degeneracy since the time-independent Schrödinger equation is a second order ordinary differential equation.

© Springer International Publishing AG 2018

P.R. Berman, *Introductory Quantum Mechanics*, UNITEXT for Physics,
https://doi.org/10.1007/978-3-319-68598-4_6

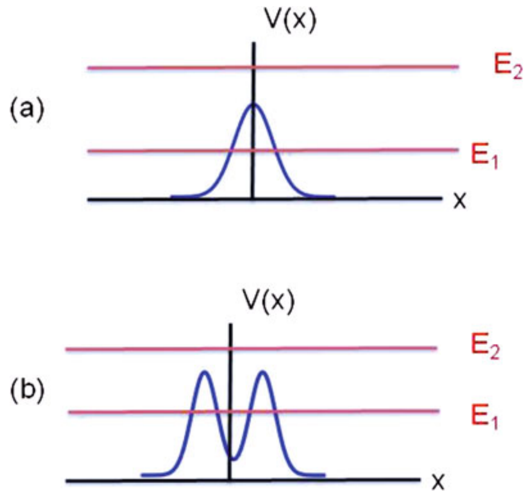

Fig. 6.1 Potential barriers

Motion in classical mechanics can be bounded or unbounded. Bounded, one-dimensional motion in classical mechanics is restricted to a finite region of space, while unbound motion can extend to either $x = \infty$ and/or $x = -\infty$. Bound states in quantum mechanics correspond to states that are, for the most part, localized to finite regions of space. In other words, a necessary condition for a bound state in quantum mechanics is that the eigenfunction associated with a bound state goes to zero as $|x| \to \infty$ (in three dimensions the eigenfunction must go to zero as $r \to \infty$). Unbound states in quantum mechanics correspond to states whose eigenfunctions do not vanish for either $x = \infty$ and/or $x = -\infty$. The eigenfunctions of the free particle do not correspond to a bound state. I now examine the classical motion and quantum-mechanical properties associated with several generic classes of one-dimensional potentials.

6.1.1 *Potentials in which* $V(x) > 0$ *and* $V(\pm\infty) \sim 0$

Potentials falling into this class are shown in Fig. 6.1. In both cases shown, there are continuous eigenenergies $E > 0$ and a two-fold degeneracy for each energy, since particles (waves) can be incident from the left or right. Were I to solve the time-independent Schrödinger equation for potentials of this type, I would find that the eigenenergies correspond to all positive energies. Classically, in case (a), a particle having energy E_1 incident from the left would be reflected by the potential. Quantum-mechanically there is some probability that the particle *tunnels* to the other side and is transmitted through the barrier. Tunneling is a wave-like phenomenon. A classical particle having energy E_2 incident from the left is always transmitted with no reflection, although its kinetic energy changes as it moves by the potential barrier. Quantum-mechanically there is some probability that the particle is reflected. For a potential that varies slowly over a de Broglie wavelength of the particle, this reflection is very small, but for a rectangular barrier it can be significant. As you shall see, the rectangular barrier case is analogous to one in which light is reflected by a dielectric slab. In case (b), classically, a particle having energy E_1 can be bound if it is located in the potential well. Quantum-mechanically there are no bound states, a particle prepared inside the well eventually tunnels out. A classical particle having energy E_1 incident from the left would always be reflected. Quantum-mechanically there is some probability that the particle is transmitted as a result of tunneling. A classical particle having energy E_2 incident from the left would always be transmitted with no reflection. Quantum-mechanically there is some probability that the particle is reflected.

6.1.2 Potentials in which $V(x) > 0$ and $V(-\infty) \sim 0$ while $V(\infty) \sim \infty$

For the potential of (Fig. 6.2) (a), a classical particle is reflected by the potential, as is a quantum wave packet incident from the left. Since a wave packet cannot be incident from the left, there is no degeneracy, although the eigenenergies are continuous. In case (b) there are no bound states quantum-mechanically, although there could be bound states classically for energy E_1, if the particle is located in the potential well.

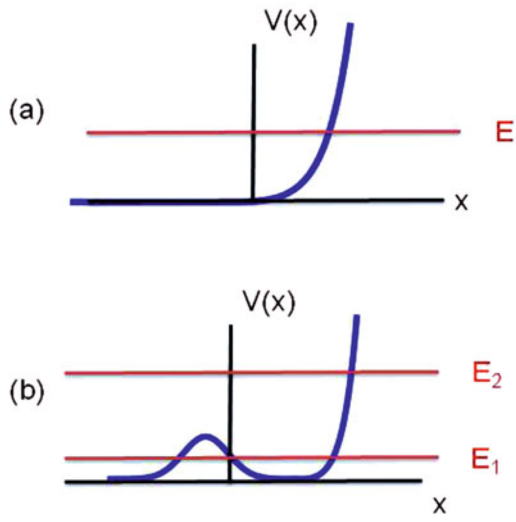

Fig. 6.2 Reflecting potentials

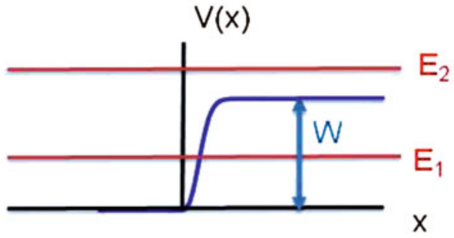

Fig. 6.3 Step potential

6.1.3 Potentials in which $V(x) > 0$ and $V(-\infty) \sim 0$ while $V(\infty) = W > 0$

In the case of a step potential (Fig. 6.3), a wave packet cannot be incident from the right if $E < W$. Therefore, for $E < W$, the eigenenergies are continuous, but there is no degeneracy. A wave packet incident from the left is totally reflected. On the other hand, for $E > W$, there are continuous eigenenergies and a two-fold degeneracy since wave packets can be incident from the left or right. Classically, a particle incident from the left is reflected if $E < W$ and transmitted with reduced kinetic energy (with no reflection) if $E > W$. Quantum mechanically there can be some reflection for a wave packet incident from the left having energy $E > W$.

6.1.4 Potentials in which $V(x) > 0$ and $V(\pm\infty) \sim \infty$

For the potentials of (Fig. 6.4), a wave packet can be incident neither from the right nor the left. The wave function must vanish as $|x| \to \infty$. In order to fit the waves in the potential and satisfy this boundary condition, the energy must take on discrete values. There is no degeneracy in this case, but there is an infinite number of discrete energies possible. Classically, any energy greater than the minimum value of the potential energy is allowed. A particle could be bound in one of the sub-wells in case (b) for energy E_1. Quantum-mechanically, there are no bound states that are localized *entirely* in only *one* sub-well.

6.1.5 Potentials in which $V(x) < 0$ and $V(\pm\infty) \sim 0$

In this case (Fig. 6.5) of a potential well, for $E > 0$, a wave packet can be incident from the left or right. Therefore, for $E > 0$, the eigenenergies are continuous, and there is a two-fold degeneracy. A wave packet incident from the left will be partially reflected and partially transmitted. There can also be *resonance* phenomena, as with

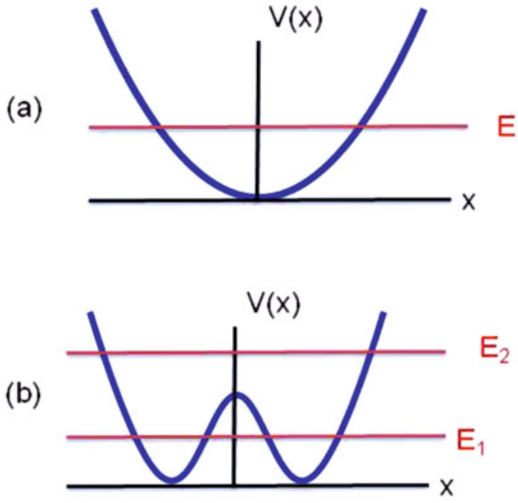

Fig. 6.4 Bound state potentials

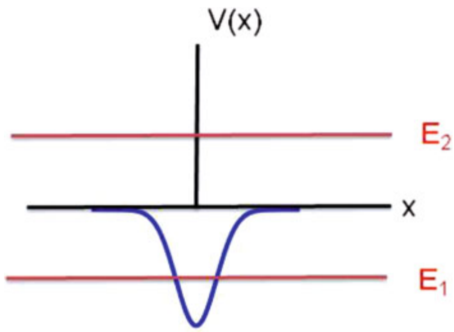

Fig. 6.5 Potential well

reflection of light from thin dielectric films. Classically there is no reflection for $E > 0$. For $E < 0$, quantum-mechanically there is no degeneracy and there is a finite number of bound states. It can be proven that there is always at least one bound state, regardless of the depth of the potential.[1] This might seem a little surprising, but, for low potential depths, the wave function extends significantly into the *classically*

[1]Somewhat more precise requirements that guarantee the existence of a bound state are $V(-\infty) = V(\infty) = V_0$ and

$$\int_{-\infty}^{\infty} [V(x) - V_0]\, dx < 0.$$

You are asked to prove this using the variational method in Problem 15.8.

forbidden regions (regions where the kinetic energy would be negative) giving rise to a large Δx and a correspondingly small Δp that is sufficiently small to prevent the particle from being freed from the well. Classically a particle having energy $E < 0$ is bound in the well.

Other types of potentials are also possible, but you should get the idea by now. In *bound state* one-dimensional problems, *there is never energy degeneracy*—the actual number of bound states (if any) depends on the details of the potential. For one-dimensional problems giving rise to continuous eigenenergies, there is two-fold degeneracy if the energy is greater than the potential as $|x| \to \infty$.

Values of x for which $E > V(x)$ correspond to the *classically allowed region* for the particle and to one for which Schrödinger's equation is

$$\frac{d^2\psi}{dx^2} = -k^2(x)\psi; \qquad k(x) = \sqrt{\frac{2m\,[E - V(x)]}{\hbar^2}} > 0. \tag{6.1}$$

If V is constant, the solutions are sines or cosines of kx. In general the solution is oscillatory in such classically allowed regions. On the other hand, values of x for which $E < V(x)$ corresponds to a *classically forbidden region* for the particle, since its kinetic energy would have to be *negative*. When $E < V(x)$, Schrödinger's equation is

$$\frac{d^2\psi}{dx^2} = \kappa^2(x)\psi; \qquad \kappa(x) = \sqrt{\frac{2m\,[V(x) - E]}{\hbar^2}} > 0. \tag{6.2}$$

For constant V, the solutions are real exponentials of $\pm\kappa x$. In general the solution is a smooth decaying function the deeper you penetrate into classically forbidden regions.

6.2 Infinite Well Potential

An important model problem in one dimension is the infinite square well potential, represented schematically in Fig. 6.6. The potential vanishes between the "walls" of

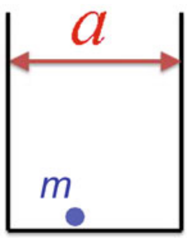

Fig. 6.6 Infinite square well potential

the potential and is infinite otherwise. This is a wonderful problem since it illustrates many of the features of bound state problems in quantum mechanics.

First, consider the classical problem. A particle having mass m is constrained to move between the walls of the potential having width a. Between the walls, the particle acts as a free particle having speed v, momentum $\mathbf{p} = \pm mv\mathbf{u}_x$ (+ if it moves to the right and − if it moves to the left) and energy $E = mv^2/2$. When the particle hits the wall, it undergoes an elastic collision in which the sign of its velocity (and momentum) is changed, but its energy remains unchanged. Since the velocity changes direction on collisions with the walls, momentum is not conserved. Also, since the velocity changes on collisions with the walls, the particle accelerates during each collision. The particle can have any kinetic energy whatsoever (the potential energy is zero inside the box), which remains constant during the particle's motion, and the position of the particle is determined precisely as it moves back and forth between the two walls.

What are the classical (time-averaged) distribution functions for this particle? The energy is fixed so the energy distribution is a Dirac delta function. For a given energy E, however, *two* possible momenta are possible,

$$\mathbf{p} = \pm\sqrt{2mE}\mathbf{u}_x \equiv p\mathbf{u}_x, \tag{6.3}$$

implying that the *time-averaged* momentum distribution in one dimension is

$$W_{\text{class}}(p) = \frac{1}{2}\left[\delta\left(p - \sqrt{2mE}\right) + \delta\left(p + \sqrt{2mE}\right)\right]. \tag{6.4}$$

On the other hand, *on average*, the particle is found with equal probability *anywhere* in the well, so the *time-averaged* spatial distribution is

$$P_{\text{class}}(x) = \frac{1}{a}. \tag{6.5}$$

Of course, the particle follows a classical trajectory given some initial condition; in other words, the probability *density* for the particle is always a Dirac delta function centered at the classical particle position. That is, the classical particle mass density is given by

$$\rho(x,t) = m\delta(x - x(t)), \tag{6.6}$$

where $x(t)$ is the position of the particle at time t.

Now let's turn to the quantum problem. The Hamiltonian for the particle when it is between the walls is just the free particle Hamiltonian,

$$\hat{H} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}. \tag{6.7}$$

As a consequence, the time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2} = E\psi_E(x) \tag{6.8}$$

in this region. I have some freedom in choosing the origin of the coordinate system. If I take the well centered at $x = 0$, the potential is symmetric about the origin and the Hamiltonian commutes with the parity operator. With this choice the eigenfunctions *must* have definite parity, since there is no energy degeneracy in this problem. On the other hand, if I take the well located between 0 and a, the Hamiltonian does not commute with the parity operator and the eigenfunctions do not possess definite parity (this is clear since the wave function must vanish for $x < 0$ in this case). Of course the eigenenergies must be the same, since the particle's energy must be independent of the choice of origin. Let's solve for the eigenfunctions and eigenenergies using both coordinate systems.

6.2.1 Well Located Between $-a/2$ and $a/2$

In this case, the potential is given by

$$V(x) = \begin{cases} 0 & |x| < a/2 \\ \infty & |x| > a/2 \end{cases}. \tag{6.9}$$

The fact that the potential is *infinite* at the wall leads us to the assumption that the eigenfunctions must vanish for $|x| \geq a/2$; that is, the particle cannot penetrate into the walls. The *boundary condition*

$$\psi_E(\pm a/2) = 0 \tag{6.10}$$

can be obtained formally by taking a finite height for the potential in the regions $|x| > a/2$, and then letting this height approach infinity. To solve Eq. (6.8) in the region $-a/2 < x < a/2$, I guess a solution. It is not difficult to show that any of

$$\sin(kx),\ \cos(kx),\ \exp(ikx)\ \ \exp(-ikx) \tag{6.11}$$

are solutions *provided*

$$k = \frac{\sqrt{2mE}}{\hbar}. \tag{6.12}$$

Since a second order differential equation has two independent solutions, I can use any *two* of the linearly independent solutions given in Eq. (6.11) that are consistent with the boundary conditions. In this case, however, there is no degeneracy and the Hamiltonian commutes with the parity operator. Thus the eigenfunctions must also be eigenfunctions of the parity operator; that is, the eigenfunctions *must* be the trigonometric solutions. The eigenfunctions fall into two classes, those having even parity and those having odd parity, namely

$$\psi_k^+(x) = N_+ \cos\left(k^+ x/2\right) \tag{6.13}$$

and

$$\psi_k^-(x) = N_- \sin\left(k^- x/2\right), \tag{6.14}$$

where the plus and minus refer to even and odd parity solutions, respectively, and the $N_\pm$ are normalization constants.

The eigenfunctions satisfy the boundary condition given in Eq. (6.10) if

$$k^+ \to k_n^+ = \frac{n\pi}{a}; \quad n = 1, 3, 5, \ldots \tag{6.15a}$$

$$k^- \to k_n^- = \frac{n\pi}{a}; \quad n = 2, 4, 6, \ldots. \tag{6.15b}$$

The $k^\pm$ values are *quantized* and, as a consequence, so is the energy

$$E \to E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2ma^2}; \quad n = 1, 2, \ldots. \tag{6.16}$$

The normalized eigenfunctions (now labeled by n rather than k) are

$$\psi_n(x) = \begin{cases} \begin{cases} \sqrt{\frac{2}{a}} \cos[n\pi x/a] & n = 1, 3, 5, \ldots \\ \sqrt{\frac{2}{a}} \sin[n\pi x/a] & n = 2, 4, 6, \ldots \end{cases} & |x| \le a/2 \\ 0 & |x| > a/2 \end{cases}, \tag{6.17}$$

where the normalization constants were obtained by demanding that

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 \, dx = \int_{-a/2}^{a/2} |\psi_n(x)|^2 \, dx = 1. \tag{6.18}$$

The first few eigenfunctions are shown in Fig. 6.7, plotted as the dimensionless quantity $\sqrt{a}\psi_n(x)$. Many of the results for the infinite well potential are generic. For example, the lowest energy eigenfunction has no nodes in the classically allowed region and is symmetric about the origin. There is one additional node in the classically allowed region for each increase in n and the eigenfunctions alternate between symmetric and antisymmetric functions. As you shall see, these features are common to all bound state problems for potentials that are an even function of x. Even if the potential is not symmetric about the origin, the same nodal structure is to be expected, although the eigenfunctions no longer correspond to states of definite parity.

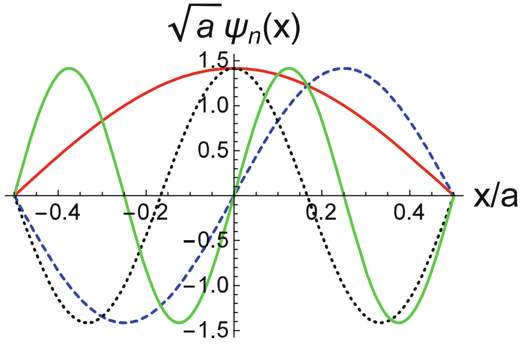

Fig. 6.7 Eigenfunctions in dimensionless units as a function of x/a for an infinite potential well centered at the origin: $n = 1$ (red, solid); $n = 2$ (blue, dashed); $n = 3$ (black, dotted); $n = 4$ (green, solid)

6.2.2 *Well Located Between 0 and a*

With this choice, the potential is

$$V(x) = \begin{cases} 0 & 0 < x < a \\ \infty & \text{otherwise} \end{cases} \tag{6.19}$$

and the boundary conditions are

$$\psi_E(0) = \psi_E(a) = 0. \tag{6.20}$$

The only solution of Eq. (6.8) in the region $0 < x < a$ that satisfies the boundary condition at $x = 0$ is of the form $\sin(kx)$ with $E = \hbar^2 k^2/2m$. To also satisfy the boundary condition that the wave function vanish at $x = a$, it is necessary that

$$k \to k_n = \frac{n\pi}{a}; \quad n = 1, 2, 3, 4, \ldots, \tag{6.21}$$

which leads to the quantized energy levels

$$E \to E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}; \quad n = 1, 2, 3, 4, \ldots; \tag{6.22}$$

as was already mentioned, the energy cannot depend on the choice of origin. The normalized eigenfunctions are

$$\psi_n(x) = \begin{cases} \sqrt{2/a}\sin[n\pi x/a] & 0 \le x \le a \\ 0 & \text{otherwise} \end{cases}. \tag{6.23}$$

Whether it is convenient to use eigenfunctions in the form of Eq. (6.17) or Eq. (6.23) depends on what properties of the solution you are investigating.

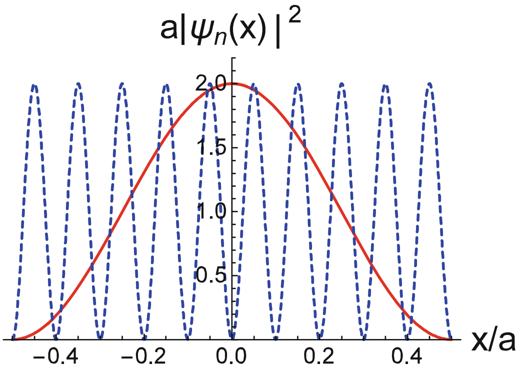

Fig. 6.8 Dimensionless probability distributions for the $n = 1$ and $n = 10$ eigenfunctions. The solid curve is for $n = 1$ and the dashed curve for $n = 10$

6.2.3 Position and Momentum Distributions

The dimensionless probability distribution $a\,|\psi_n(x)|^2$ is shown in Fig. 6.8 for $n = 1$ and $n = 10$ for the well located between $-a/2$ and $a/2$. You see that, for $n = 1$, the function is "bell-shaped," but for $n = 10$, there are many oscillations. If I average these oscillations for large n, I find that $\left\langle |\psi_n(x)|^2 \right\rangle = 1/a$, in agreement with the classical distribution given in Eq. (6.5), suggesting that $|\psi_n(x)|^2$ can be interpreted as a probability distribution. This is a bit of a swindle, however, since, in a state of given n, the quantum probability distribution is very different from the classical one. The classical distribution is a delta function centered at the classical particle position, while there are many places in the quantum distribution where the particle *cannot be found at all*. To get a *true* classical limit, you must take a superposition of a large number of quantum states to form a wave packet that will bounce back and forth between the walls with minimal spreading, simulating the classical particle motion. On the other hand, I have uncovered an important link between the classical and quantum problem. In the limit of large quantum numbers (high n), the quantum distribution, *averaged over oscillations in the classically allowed region* is approximately equal to the *time-averaged* classical particle density for a particle having an energy equal to that associated with the quantum state n.

The situation in momentum space is a bit closer to the classical picture. The eigenfunctions can be expanded as

$$\psi_n(x) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{\infty} dp \Phi_n(p) e^{ipx/\hbar}, \tag{6.24}$$

where the expansion coefficients $\Phi_n(p)$ are simply the Fourier transform of the spatial ones

$$\Phi_n(p) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{\infty} dx \psi_n(x) e^{-ipx/\hbar}. \tag{6.25}$$

I will assume that $|\Phi_n(p)|^2$ corresponds to the momentum distribution associated with the eigenfunction $\psi_n(x)$. Since the *momentum* distribution is independent of the choice of coordinates, I can choose the wave functions given by Eq. (6.23) since it allows me to get an expression for all n. Using Eq. (6.23) for $\psi_n(x)$, I calculate the momentum eigenfunctions as

$$\begin{aligned}\Phi_n(p) &= \frac{1}{(2\pi\hbar)^{1/2}} \sqrt{\frac{2}{a}} \int_0^a dx \sin(n\pi x/a)\, e^{-ipx/\hbar} \\ &= -\frac{n}{\pi\sqrt{p_c}} \frac{[1-(-1)^n \exp(-i\pi p/p_c)]}{(p/p_c)^2 - n^2},\end{aligned} \tag{6.26}$$

where

$$p_c = \pi\hbar/a. \tag{6.27}$$

The momentum distribution is then given by

$$|\Phi_n(p)|^2 = \frac{2n^2}{\pi^2 p_c} \frac{1-(-1)^n \cos(\pi p/p_c)}{\left[(p/p_c)^2 - n^2\right]^2}, \tag{6.28}$$

valid for any integer $n \geq 1$.

In Fig. 6.9, the dimensionless momentum distribution $p_c\, |\Phi_n(p)|^2$ is plotted as a function of p/p_c for $n = 1, 2, 10$. For $n = 1$, the distribution is a smooth curve having HWHM $\Delta p_{1/2}(n = 1)$ approximately equal to $1.19 p_c$. For $n \geq 2$, the distribution consists of two peaks whose centers are separated by

$$\delta p_n = 2np_c = 2n\pi\hbar/a. \tag{6.29}$$

In the problems you are asked to show that, for $n \gg 1$, the height of each peak, $p_c\, |\Phi_n(np_c)|^2$, approaches a value equal to $1/4$ and the HWHM of each peak approaches a value equal to $\Delta p_{1/2} \approx 2.79 p_c/\pi = 2.79\hbar/a$, *independent of* n. You can think of the width of each peak as being determined from the uncertainty principle. Since Δx equals $a/\sqrt{12}$ for large n (see below), the *magnitude* of the momentum cannot be determined to better than $\hbar/(2\Delta x) = \sqrt{3}\hbar/a = 1.73\hbar/a$.

For large n the distribution mirrors that of the classical distribution given in Eq. (6.4), since it consists of two peaks centered at

$$p_n = \pm(n\pi\hbar/a) = \pm\sqrt{2mE_n}, \tag{6.30}$$

as in the classical case. The peaks do *not* approach delta functions as in the classical case, but $\Delta p_{1/2}/\delta p_n \sim 0$ as $n \to \infty$.

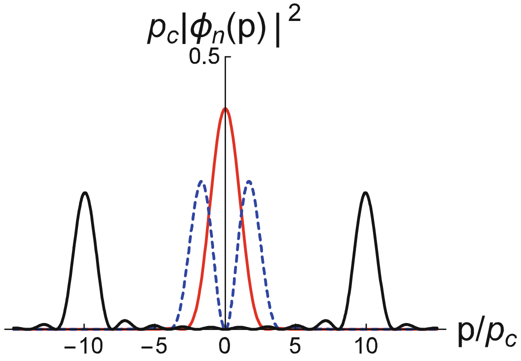

Fig. 6.9 Dimensionless eigenfunction momentum probability distributions as a function of p/p_c for $n = 1$ (solid single-peaked curve), $n = 2$ (dashed curve), and $n = 10$ (solid double-peaked curve)

It is not difficult to calculate the variance in position and momentum associated with each eigenfunction,

$$\Delta x_n^2 = \int_{-a/2}^{a/2} x^2 |\psi_n(x)|^2 \, dx = \left(\frac{1}{12} - \frac{1}{2n^2\pi^2} \right) a^2; \tag{6.31a}$$

$$\Delta p_n^2 = \int_{-\infty}^{\infty} p^2 |\Phi_n(p)|^2 \, dp = \hbar^2 n^2 \pi^2 / a^2, \tag{6.31b}$$

implying that

$$\Delta x_n \Delta p_n = \hbar \left(\frac{n^2\pi^2}{12} - \frac{1}{2} \right)^{1/2} \geq 0.568\hbar. \tag{6.32}$$

The uncertainty Δx_n grows with increasing n because the wave function becomes more spread out over the well. In the limit that $n \gg 1$, $\Delta x_n \sim a/\sqrt{12}$, the standard deviation of the classical probability distribution, $P_{\text{class}}(x) = 1/a$. Although the momentum distribution consists of two very sharp peaks for large values of n, Δp_n^2 grows with increasing n since the separation of the peaks is proportional to n for large n. A similar result holds for the classical momentum distribution with increasing energy.

6.2.4 Quantum Dynamics

To remind you that the solution of the time-independent Schrödinger equation allows you to calculate the quantum dynamics, I consider an initial state wave function (for a well centered at $x = 0$)

$$\psi(x,0) = \begin{cases} Ne^{-x^2/2b^2} & |x| \leq a/2 \\ 0 & \text{otherwise} \end{cases}, \tag{6.33}$$

where $b \ll a$ and N is a normalization factor given by[2]

$$N = \left(\int_{-a/2}^{a/2} dx e^{-x^2/b^2} \right)^{-1/2} \approx \frac{1}{\sqrt{b\pi^{1/2}}}. \tag{6.34}$$

The particle has an average momentum of zero and is localized at the center of the well with a position uncertainty of order b. The goal is to calculate $\psi(x,t)$.

Without going into the details of the exact solution, I can get a qualitative picture of what is going to happen. In other words, I can ask questions such as "How many eigenfunctions are needed in the expansion of the initial state wave function?", "When does the particle know that it was contained in a potential well?", "Does the particle ever return to its initial shape?"

The uncertainty in the momentum of the particle is $\Delta p \approx \hbar/\sqrt{2}b$ and the energy associated with this uncertainty is $\Delta E = \hbar^2/4mb^2$. As a consequence, I would expect to need to include energies at least equal to ΔE in the sum over eigenfunctions if I am to correctly approximate the initial state wave function. In other words, for some $n_{\max}$, I can approximate the dimensionless wave function as

$$\sqrt{a}\psi_{\text{app}}(x,0) = \sum_{n=1}^{n_{\max}} a_n \psi_n(x), \tag{6.35}$$

where

$$a_n = \begin{cases} \sqrt{2} \int_{-a/2}^{a/2} dx\, Ne^{-x^2/2b^2} \cos \frac{n\pi x}{a} & n \text{ odd} \\ \sqrt{2} \int_{-a/2}^{a/2} dx\, Ne^{-x^2/2b^2} \sin \frac{n\pi x}{a} = 0 & n \text{ even} \end{cases}. \tag{6.36}$$

I would expect the wave function (6.35) to be a good approximation to the exact initial wave function provided

$$n_{\max} \gg \sqrt{\frac{2ma^2 \Delta E}{\pi^2 \hbar^2}} = \frac{a}{\sqrt{2}\pi b}. \tag{6.37}$$

With $a/b = 10$ ($a/\sqrt{2}\pi b \approx 2.25$), $\sqrt{a}\psi_{\text{app}}(x,0)$ is shown in Fig. 6.10 for $n_{\max} = 1, 5, 9$, and compared with $\sqrt{a}\psi(x,0)$. For $n_{\max} = 9$, the two curves pretty much overlap.

As time progresses, the wave function spreads and $\Delta x(t)$, the standard deviation at time t, increases. For large times when $\Delta pt/m \gg \Delta x(0)$, $\Delta x(t) \approx \Delta pt/m$, so the "particle" spreads to the wall in a time of order

[2] In principle, the wave function in Eq. (6.33) should be multiplied by a factor such as $\cos(\pi x/a)$ to insure that $\psi(x,0)$ satisfies the correct boundary conditions at $x = \pm a/2$. However, if $b \ll a$, $e^{-x^2/2b^2}\cos(\pi x/a) \approx e^{-x^2/2b^2}$ for $-a/2 < x < a/2$. For this reason the $\cos(\pi x/a)$ factor has been omitted.

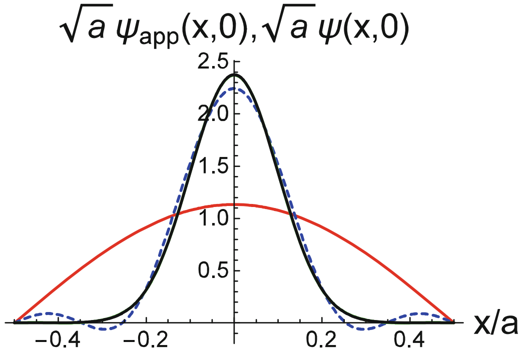

Fig. 6.10 Wave function $\psi(x, 0)$ in dimensionless units as a function of x/a. The solid, black curve is the exact wave function given by Eq. (6.33) with $b/a = 0.1$. The other curves are approximations to the wave function calculated using Eq. (6.35) for different values of $n_{\max}$; the red, solid curve corresponds to $n_{\max} = 1$, the blue, dashed curve to $n_{\max} = 5$, and the green, solid curve to $n_{\max} = 9$. The $n_{\max} = 9$ curve is barely distinguishable from the original wave function

$$t_{sp} = \frac{a}{2\Delta v} = \frac{mab}{\sqrt{2}\hbar}, \tag{6.38}$$

where $\Delta v = \Delta p/m$ is the speed uncertainty in the initial packet. Note that t_{sp} depends inversely on $\hbar$ so the particle reaching the wall is a quantum effect related to wave-packet spreading (in other words, $t_{sp} \sim \infty$ as $\hbar \sim 0$). The time t_{sp} is the characteristic time it takes for the initial wave packet to acquire a width of order a as a result of spreading. It is the time need for the particle to "know" it was confined to the infinite potential well.

I can also simulate a classical particle moving back and forth in the well by taking as an initial state wave function

$$\psi(x, 0) = \begin{cases} Ne^{-x^2/2b^2} e^{ik_0 x} & -a/2 \le x \le a/2 \\ 0 & \text{otherwise} \end{cases}, \tag{6.39}$$

where $b \ll a$ and N is given by Eq. (6.34). The factor $e^{ik_0 x}$ leads to an initial average momentum of the packet equal to $p_0 = \hbar k_0 \mathbf{u}_x$. The momentum spread is still of order $\Delta p \approx \hbar/\sqrt{2}b$; however, now the particle, which might have thought it was free, is in for a rude awakening when it strikes the wall of the well in a time of order $a/2v_0$, where $v_0 = p_0/m$. The range Δn of energy eigenfunctions needed to construct this packet is still of order $a/2\pi b$, but the states are now centered about the integer closest to

$$n_0 = \frac{p_0 a}{\pi\hbar} = \frac{p_0}{p_c}, \tag{6.40}$$

obtained by setting $E_{n_0} = mv_0^2/2$. The particle makes of order

$$t_{sp}/\left(\frac{a}{v_0}\right) = t_{sp}/\left(\frac{ma}{p_0}\right) = \frac{bp_0}{\sqrt{2}\hbar} = \frac{\sqrt{2}\pi b}{\lambda_{dB}} \tag{6.41}$$

wall collisions before spreading of the packet is significant ($\lambda_{dB} = h/p_0$ is the average de Broglie wavelength of the initial packet). As long as $b/\lambda_{dB} \gg 1$, the quantum wave packet can be considered to represent a classical particle for times $t \ll t_{sp}$.

There is one additional interesting feature in this problem. If I write the general form for the wave function at time t as

$$\psi(x,t) = \sum_{n=1}^{\infty} a_n e^{-in^2\omega_1 t}\psi_n(x), \tag{6.42}$$

where

$$\omega_1 = \frac{E_1}{\hbar} = \frac{\hbar\pi^2}{2ma^2}, \tag{6.43}$$

it is clear that the initial wave packet is reproduced at integral multiples of the *revival time*

$$t_r = \frac{2\pi}{\omega_1} = \frac{4ma^2}{\hbar\pi}. \tag{6.44}$$

Such *quantum revivals* are a purely quantum effect since the revival time t_r goes to infinity as $\hbar$ goes to zero. Although a little harder to prove (see problems), quantum revivals $[|\psi(x,t)|^2 = |\psi(x,0)|^2]$ occur for times t that are integral multiples of $t_r/8$ if the initial wave function is symmetric about the origin, for times t that are integral multiples of $t_r/4$ if the initial wave function is antisymmetric about the origin. Moreover, regardless of the functional form of the initial wave function, $|\psi(-x,t)|^2 = |\psi(x,0)|^2$ for times t that are half-integral multiples of t_r.

6.3 Piecewise Constant Potentials

I now examine problems involving *piecewise constant potentials*. In other words, I look at problems in which the potential is constant in several regions, but undergoes point jump discontinuities between regions. An analogous problem in optics is transmission and reflection of light at a dielectric surface, in which the index of refraction is constant on either side of the dielectric interface, but undergoes a point jump discontinuity at the interface. Of course, no physical boundary can be infinitely sharp. In the optical case, the change in index is assumed to occur over a distance small compared with a wavelength, which can be satisfied quite easily using polished surfaces. In quantum mechanics, it is assumed that the change in the potential occurs over a distance that is small compared to a de Broglie

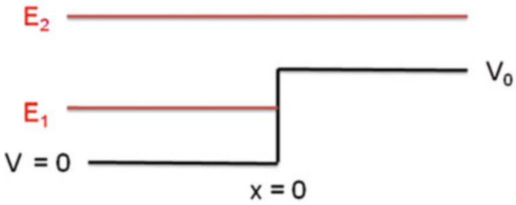

Fig. 6.11 Step potential

wavelength, a condition that is much harder to achieve experimentally. Let's forget about these complications for the moment and begin a systematic attack on this problem. I concentrate on solutions of the time-independent Schrödinger equation, but discuss wave packet dynamics as well. In problems involving reflection and transmission, I use the probability current density to obtain the reflection and transmission coefficients. I will not be concerned about normalizing the wave functions in problems involving reflection and transmission; I simply calculate the ratio of transmitted and reflected probability current densities to the incident probability current density.

6.3.1 *Potential Step*

Consider the potential step shown in Fig. 6.11,

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases} . \tag{6.45}$$

There is a point jump discontinuity in the potential at $x = 0$, but, as long as the potential contains no singularities or infinities, both the wave function and its derivative are continuous at all points, since they are solutions of a well-behaved, second order, linear differential equation. To obtain the eigenfunctions, I solve Schrödinger's equation for $x < 0$ and for $x > 0$ and then equate the wave functions of the two solutions and their derivatives at $x = 0$. On physical grounds, the continuity of the wave function is consistent with the idea that the probability density must be a single valued function.

The procedure I follow for the step potential can be used in any problem involving piecewise constant potentials. That is, I solve the Schrödinger equation in each region of constant potential and use the continuity of the wave function and its derivative to connect the solutions. Additional boundary conditions are often needed for the solutions as $|x| \to \infty$. For the potential step, I consider $E < V_0$ and $E > V_0$ separately.

6.3.1.1 $E < V_0$

In the classical problem, a particle that approaches the barrier is reflected with the same speed. In the quantum-mechanical problem, I could simulate the classical problem by sending a wave packet towards the barrier. When I discuss scattering theory in Chap. 17, you will see that the wave packet actually penetrates into the barrier, but is then totally reflected with a *time delay* that depends on $(V_0 - E)/E$. In this chapter, I consider the time-independent problem only and calculate the reflection coefficient using the probability current density.

I need to solve the Schrödinger equation for $x < 0$ and for $x > 0$ and then match the wave functions of the two regions and their derivatives at $x = 0$. I know already that the eigenvalues are continuous and there is no degeneracy. For region I, in which $x < 0$ and $V(x) = 0$,

$$\frac{d^2\psi_{IE}(x)}{dx^2} = -k_E^2\psi_{IE}(x) \tag{6.46}$$

where

$$k_E = \frac{\sqrt{2mE}}{\hbar} > 0. \tag{6.47}$$

The general solution of this equation is exponentials or sines and cosines. It is better to choose exponentials since it will then be possible to interpret the results in terms of an incident and reflected probability current. Although there is no degeneracy I must take the most general possible solution of Eq. (6.46) or I will not be able to match the *two* boundary conditions at $x = 0$ for the continuity of the wave function and its derivative. Thus I take

$$\psi_{IE}(x) = Ae^{ik_Ex} + Be^{-ik_Ex}; \qquad x < 0. \tag{6.48}$$

For region II, in which $x > 0$ and $V(x) = V_0$, Schrödinger's equation is

$$\frac{d^2\psi_{IIE}(x)}{dx^2} = \kappa_E^2\psi_{IIE}(x), \tag{6.49}$$

where

$$\kappa_E = \frac{\sqrt{2m(V_0 - E)}}{\hbar} > 0. \tag{6.50}$$

The possible solutions are $e^{\pm\kappa_Ex}$ but I must reject the $+$ exponential since it blows up for large x. That is, the boundary condition requiring the wave function to be finite at all points in space requires me to reject a solution of the form e^{κ_Ex} as $x \to \infty$. Thus, I take

$$\psi_{IIE}(x) = Ce^{-\kappa_Ex}; \qquad x > 0. \tag{6.51}$$

Combining Eqs. (6.48) and (6.51), I find that the eigenfunction corresponding to an energy $0 < E < V_0$ is

$$\psi_E(x) = \begin{cases} Ae^{ik_E x} + Be^{-ik_E x} & x < 0 \\ Ce^{-\kappa_E x} & x > 0 \end{cases} . \tag{6.52}$$

It is possible to normalize this solution if some type of convergence factor is introduced (see problems), but the normalization is unimportant for our considerations.

Equating the wave function and its derivative at $x = 0$, I obtain the two equations

$$A + B = C; \tag{6.53a}$$

$$ik_E (A - B) = -\kappa_E C, \tag{6.53b}$$

from which I find

$$\frac{B}{A} = \frac{k_E - i\kappa_E}{k_E + i\kappa_E}; \tag{6.54a}$$

$$\frac{C}{A} = \frac{2k_E}{k_E + i\kappa_E}. \tag{6.54b}$$

What do these ratios mean?

To interpret them, I look at the probability current density associated with *each* component of the eigenfunction for $x < 0$. The probability current density [see Eq. (5.139)] associated with the $Ae^{ik_E x}$ part of the eigenfunction is $J_i = v_E |A|^2$ while that associated with the $Be^{-ik_E x}$ part is $J_r = -v_E |B|^2$, where $v_E = \hbar k_E/m$ and the i and r subscripts stand for "incident" and "reflected," respectively. I interpret

$$R = \frac{B}{A} \tag{6.55}$$

as an *amplitude reflection coefficient* and

$$\mathcal{R} = |R|^2 = -\frac{J_r}{J_i} = \frac{v_E |B|^2}{v_E |A|^2} = \left|\frac{B}{A}\right|^2 = 1 \tag{6.56}$$

as an *intensity reflection coefficient*. Since $\mathcal{R} = 1$, the wave is totally reflected. The probability current density *inside* the potential step vanishes since the wave function is real, but the quantity

$$\left|\frac{C}{A}\right|^2 = \frac{4k_E^2}{\kappa_E^2 + k_E^2} = \frac{4E}{V_0} \tag{6.57}$$

turns out to be a measure of the distance that a wave packet penetrates into the potential step before it is totally reflected (you have to solve the scattering problem to see this, as I do in Chap. 17). The problem is analogous to total reflection of light by a lossless plasma, when the frequency of the light is below the plasma frequency.

In the limit that $V_0 \to \infty$, $C/A \sim 0$, consistent with the assumption that the wave function vanishes in extended regions where there is an infinite potential. Moreover, as $V_0 \to \infty$, $B/A \sim -1$ in Eq. (6.54a), which implies a phase change of π on reflection. Therefore, as $V_0 \to \infty$, Eq. (6.52) reduces to

$$\psi_E(x) \sim \begin{cases} 2iA \sin(k_E x) & x < 0 \\ 0 & x > 0 \end{cases}. \tag{6.58}$$

The eigenfunctions are now *standing waves*, with a node at $x = 0$. The analogous situation for electromagnetic radiation is reflection at a perfect metal, where the tangential component of the electric field must vanish at the surface.

Another interesting limit occurs for $E \approx V_0$ ($E = V_0 - \epsilon$, with $0 < \epsilon \ll V_0$), for which $B/A \sim 1$, $C/A \sim 2$, and

$$\psi_E(x) \sim \begin{cases} 2A \cos(k_E x) & x < 0 \\ 2Ae^{-\kappa_E x}; \quad \kappa_E = \frac{\sqrt{2m\epsilon}}{\hbar^2}; & x > 0 \end{cases}. \tag{6.59}$$

In this limit the intensity reflection coefficient is still equal to unity, but there is no phase change on reflection. The wave function penetrates deeply into the potential step. In the classically allowed region the wave functions is a standing wave with an *antinode* at $x = 0$. If a wave packet having fairly well-defined energy $E \approx V_0$ is incident on the potential step, there is a long time delay before the packet is totally reflected.

6.3.1.2 $E > V_0$

In the classical problem, a particle approaches the potential step and is transmitted with a lower speed. There is no reflection in the classical problem. In the quantum-mechanical problem, a wave packet incident on the potential step is partially transmitted and partially reflected, with the reflection coefficient depending on $(E - V_0)/E$. The eigenenergies are continuous and there is a two-fold degeneracy.

For region I, in which $x < 0$,

$$\frac{d^2\psi_{IE}(x)}{dx^2} = -k_E^2 \psi_{IE}(x) \tag{6.60}$$

as before, but for region II, in which $x > 0$, Eq. (6.49) is replaced by

$$\frac{d^2\psi_{IIE}(x)}{dx^2} = -k_E'^2 \psi_{IIE}(x) \tag{6.61}$$

where

$$k_E' = \frac{\sqrt{2m(E - V_0)}}{\hbar} > 0. \tag{6.62}$$

You might think that I need to try a solution of the form

$$\psi_E(x) = \begin{cases} Ae^{ik_E x} + Be^{-ik_E x} & x < 0 \\ Ce^{ik'_E x} + De^{-ik'_E x} & x > 0 \end{cases}; \tag{6.63}$$

however, I will run into problems with such a solution. There are four unknowns in this equation. Using the boundary conditions at $x = 0$ gives two constraints (continuity of the wave function and its derivative) and normalization a third, but I am one short since I need four constraints. The reason for this dilemma is that there is a two-fold degeneracy in this problem. I must take two *independent* solutions for each energy. One way of doing this is to arbitrarily set one of the coefficients equal to zero in each of two separate solutions.

I do this in a manner that allows me simulate waves incident from the left or right; that is, I take

$$\psi_E^L(x) = \begin{cases} A_L e^{ik_E x} + B_L e^{-ik_E x} & x < 0 \\ C_L e^{ik'_E x} & x > 0 \end{cases}, \tag{6.64}$$

corresponding to a wave incident from the left and

$$\psi_E^R(x) = \begin{cases} C_R e^{-ik_E x} & x < 0 \\ A_R e^{-ik'_E x} + B_R e^{ik'_E x} & x > 0 \end{cases}, \tag{6.65}$$

corresponding to a wave incident from the right. These are two independent solutions for each energy $E > V_0$. Of course, any two, linearly independent combinations of Eqs. (6.64) and (6.65) could be used as well. I consider only the solution for the wave incident from the left [Eq. (6.64)] and drop the L superscript. The solutions (6.64) and (6.65) contain plane wave *components*, but these eigenfunctions are *not* plane waves, even if they extend over all space. As I have stressed, each potential has its own set of eigenfunctions; the only potential allowing for plane wave eigenfunctions is $V = 0$ (or a constant) in all space.

Matching the wave functions in the two regions and their derivatives at $x = 0$, I find

$$A + B = C; \tag{6.66a}$$

$$k_E (A - B) = k'_E C, \tag{6.66b}$$

from which I can obtain

$$R = \frac{B}{A} = \frac{k_E - k'_E}{k_E + k'_E}; \tag{6.67a}$$

$$T = \frac{C}{A} = \frac{2k_E}{k_E + k'_E}, \tag{6.67b}$$

as the amplitude reflection and transmission coefficients, respectively. The probability current density associated with Ae^{ik_Ex} is $J_i = v_E|A|^2$, that associated with Be^{-ik_Ex} is $J_r = -v_E|B|^2$, while that associated with $Ce^{ik'_Ex}$ is $J_t = v'_E|C|^2$, where $v_E = \hbar k_E/m$, $v'_E = \hbar k'_E/m$, and the t subscript stand for "transmitted." Thus

$$\mathcal{R} = |R|^2 = -\frac{J_r}{J_i} = \frac{v_E}{v_E}\left|\frac{B}{A}\right|^2 = \left(\frac{k_E - k'_E}{k_E + k'_E}\right)^2 = \left(\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}}\right)^2 \tag{6.68}$$

is the (intensity) reflection coefficient and

$$\begin{aligned}\mathcal{T} = |T|^2 = \frac{J_t}{J_i} = \frac{v'_E}{v_E}\left|\frac{C}{A}\right|^2 &= \frac{k'_E}{k_E}\left(\frac{2k_E}{k_E + k'_E}\right)^2 \\ &= \frac{4k_E k'_E}{\left(k_E + k'_E\right)^2} = \frac{4\sqrt{E}\sqrt{E - V_0}}{\left(\sqrt{E} + \sqrt{E - V_0}\right)^2}\end{aligned} \tag{6.69}$$

is the (intensity) transmission coefficient. The fact that

$$\mathcal{R} + \mathcal{T} = 1, \tag{6.70}$$

is a statement of conservation of probability.

It is interesting to note that both $\mathcal{R}$ and $\mathcal{T}$ are independent of $\hbar$. That is, even if I take a classical limit in which $\hbar \to 0$, I do not recover the classical result of $\mathcal{R} \to 0$. The reason is simple. For the classical limit to hold, *changes* in the potential must occur on a length scale that is large compared with the de Broglie wavelength. Since the potential changes abruptly this is not possible. If the potential rose smoothly over a distance large compared with the de Broglie wavelength, there would be virtually no reflection as $\hbar \to 0$. In fact, for a smooth potential step of the form

$$V(x) = \frac{V_0}{1 + e^{-x/a}}, \tag{6.71}$$

where $a > 0$ is the length scale of the step, it is possible to solve Schrödinger's equation exactly in terms of hypergeometric functions and to show analytically that the reflection coefficient is[3]

$$\mathcal{R} = \left[\frac{\sinh\left[\pi\left(k_E - k'_E\right)a\right]}{\sinh\left[\pi\left(k_E + k'_E\right)a\right]}\right]^2, \tag{6.72}$$

which reduces to Eq. (6.68) when $k_E a = 2\pi a/\lambda_{dB} \ll 1$, but varies as $\exp\left(-4\pi k'_E a\right) \sim 0$ in the limit that a is finite and $\hbar \to 0$.

---

[3] See L. D Landau and E. M. Lifshitz, *Quantum Mechanics, Non-Relativistic Theory* (Pergamon Press, London, 1958), pp. 75–76.

The quantum step potential problem with $E > V_0$ is analogous to the reflection of light at a dielectric. As long as the interface is sharper than a wavelength, there is *always* a reflected wave. For normal incidence from vacuum to a medium having index of refraction n, the ratio of reflected to incident pulse *amplitudes* is

$$R = \left.\frac{B}{A}\right|_{\text{light}} = \frac{1-n}{1+n} \tag{6.73}$$

and the speed of light in the dielectric is c/n. This agrees with Eq. (6.67a) if I set

$$n \to n_{\text{eff}} = \sqrt{\frac{E-V_0}{E}} = \sqrt{1-\frac{V_0}{E}} < 1 \tag{6.74}$$

Thus, even though the *particle* speed *decreases*, the effective *index* is less than unity. The analogue with reflection at a dielectric is not exact, although the results take on the same form. Changes in the incident wavelength for light do not seriously affect the index of refraction, but the effective index depends in a significant way on the incident energy for matter waves.

In solving the Schrödinger equation for both $E < V_0$ and $E > V_0$, I automatically determined the eigenergies and the eigenfunctions. For $E < V_0$, I found that any energy in the range $0 < E < V_0$ gives rise to a solution and that the eigenfunctions are nondegenerate. For $E > V_0$, I found that any energy gives rise to a doubly-degenerate solution.

6.3.2 *Square Well Potential*

Now I turn my attention to the square well potential shown in Fig. 6.12 for which

$$V(x) = \begin{cases} -V_0 < 0 & |x| < a/2 \\ 0 & |x| > a/2 \end{cases}. \tag{6.75}$$

I consider $E < 0$ and $E > 0$ separately. I must solve the Schrödinger equation in three regions, $x < -a/2$, $-a/2 < x < a/2$, $x > a/2$, and equate the wave functions of the solutions and their derivatives at $x = -a/2$ and $x = a/2$.

6.3.2.1 $E < 0$

In the classical problem, a particle is always bound in the well for $E < 0$. In the quantum mechanics problem, you will see that there is always at least one bound state. However, the wave function penetrates into the classically forbidden regime.

You might think that there is no bound state for sufficiently small well depths based on the following argument. Since Δx is of order a, Δp is of order $\hbar/a$,

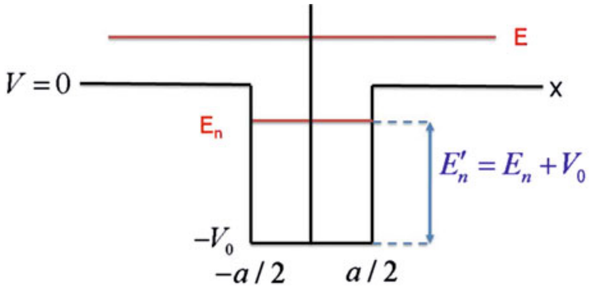

Fig. 6.12 Square well potential. There are unbound eigenfunctions for all positive energies and a finite number of bound states E_n for negative energies. The number of bound states is equal to the integer value of $(1 + \beta/\pi)$, where $\beta^2 = 2mV_0a^2/\hbar^2$

corresponding to an energy of $\hbar^2/2ma^2$. Therefore if $V_0 < \hbar^2/2ma^2$, the well is not deep enough to bind the particle. You will see what is wrong with this argument after I analyze the problem in detail.

For $E < 0$, the eigenenergies are discrete and there is no degeneracy. I can simplify the problem somewhat by noting that the Hamiltonian commutes with the parity operator. Therefore the energy eigenfunctions are guaranteed to be simultaneous eigenfunctions of the parity operator. The boundary conditions are such that the wave function must vanish as x approaches $\pm\infty$. The even parity solutions of Schrödinger's equation satisfying the boundary conditions at $x = \pm\infty$ are

$$\psi_E^+(x) = \begin{cases} B^+ e^{\kappa_E^+ x} & x < -a/2 \\ A^+ \cos\left(k_E'^+ x\right) & -a/2 < x < a/2 \\ B^+ e^{-\kappa_E^+ x} & x > a/2 \end{cases} \tag{6.76}$$

and the odd parity solutions are

$$\psi_E^-(x) = \begin{cases} B^- e^{\kappa_E^- x} & x < -a/2 \\ A^- \sin\left(k_E'^- x\right) & -a/2 < x < a/2 \\ -B^- e^{-\kappa_E^- x} & x > a/2 \end{cases}, \tag{6.77}$$

where

$$k_E'^{\pm} = \frac{\sqrt{2mE'^{\pm}}}{\hbar} > 0, \tag{6.78}$$

$$\kappa_E^{\pm} = \frac{\sqrt{-2mE^{\pm}}}{\hbar} > 0, \tag{6.79}$$

$$E'^{\pm} = \left(E^{\pm} + V_0\right), \tag{6.80}$$

m is the particle mass, and $+$ $(-)$ corresponds to even (odd) parity. The energy $E'^{\pm}$ is the *difference* between $E^{\pm}$ and the energy $-V_0$ at the bottom of the well (see Fig. 6.12).

By choosing the energy eigenfunctions to be simultaneous eigenfunctions of the parity operator, I guarantee that if I satisfy the boundary conditions on the wave function and its derivative at $x = a/2$, they are automatically satisfied at $x = -a/2$. Matching the wave functions their derivatives at $x = a/2$, I find

$$A^{+} \cos\left(\frac{k_E'^{+} a}{2}\right) = B^{+} \exp\left(-\frac{\kappa_E^{+} a}{2}\right) \tag{6.81a}$$

$$A^{+} k_E'^{+} \sin\left(\frac{k_E'^{+} a}{2}\right) = B^{+} \kappa_E^{+} \exp\left(-\frac{\kappa_E^{+} a}{2}\right) \tag{6.81b}$$

for the even parity solutions and

$$A^{-} \sin\left(\frac{k_E'^{-} a}{2}\right) = B^{-} \exp\left(-\frac{\kappa_E^{-} a}{2}\right) \tag{6.82a}$$

$$A^{-} k_E'^{-} \cos\left(\frac{k_E'^{-} a}{2}\right) = -B^{-} \kappa_E^{-} \exp\left(-\frac{\kappa_E^{-} a}{2}\right) \tag{6.82b}$$

for the odd parity solutions.

Equations (6.81) and (6.82) are typical of the type encountered in solving bound state problems for piecewise constant potentials. They are homogeneous equations with the same number of equations as unknowns. The only way to have non-trivial solutions of such equations is for the determinant of the coefficients to vanish. In solving the determinant equation, you find solutions for only *specific values of the energy*. This is why bound state motion leads to discrete or quantized eigenenergies.

Instead of setting the determinant of the coefficients in Eqs. (6.81) and (6.82) equal to zero, it is simpler to divide the equations to obtain

$$\tan\left(\frac{k_E'^{+} a}{2}\right) = \frac{\kappa_E^{+}}{k_E'^{+}} \tag{6.83}$$

for the even parity solutions and

$$\tan\left(\frac{k_E'^{-} a}{2}\right) = -\frac{k_E'^{-}}{\kappa_E^{-}} \tag{6.84}$$

for the odd parity solutions. Note that $k_E'^{-} = 0$ is not an acceptable odd parity solution [even though it is a solution of Eq. (6.84)] since it is not a solution of Eqs. (6.82). In other words, Eq. (6.84) gives the solutions to Eqs. (6.82) provided $k_E'^{-} \neq 0$.

I define dimensionless quantities

$$\beta^2 = \frac{2mV_0}{\hbar^2}a^2, \tag{6.85}$$

$$\left(y^{\pm}\right)^2 = \left(k_E'^{\pm}\right)^2 a^2, \tag{6.86}$$

such that

$$\kappa_E^{\pm} a = \sqrt{\frac{2m\left(V_0 - E'^{\pm}\right)}{\hbar^2}}a = \sqrt{\beta^2 - \left(y^{\pm}\right)^2}. \tag{6.87}$$

The quantity β^2 is a dimensionless measure of the strength of the well that we will encounter often. The condition determining the even parity eigenenergies is

$$\tan\left(\frac{y^+}{2}\right) = \frac{\kappa_E^+}{k_E'^+} = \sqrt{\frac{\beta^2}{\left(y^+\right)^2} - 1} > 0, \tag{6.88}$$

while the condition for the odd parity eigenfunctions is

$$\tan\left(\frac{y^-}{2}\right) = -\frac{1}{\sqrt{\frac{\beta^2}{(y^-)^2} - 1}} < 0. \tag{6.89}$$

Equations (6.88) and (6.89) can be solved graphically. The graphical solution for the even parity solution, Eq. (6.88), is shown in Figs. 6.13 and 6.14 for $\beta = 0.5$ and $\beta = 20$, respectively. As you can see there is always *at least one solution*, irrespective of the value of β. Why does the uncertainty principle argument given above fail? For $\beta \ll 1$, the value of $\kappa_E^+ a$ becomes small and the eigenfunction penetrates a long distance into the classically forbidden region. Thus the estimate that $\Delta x = a$ is wrong—I should use $\Delta x = \left(\kappa_E^+\right)^{-1} \approx a/\beta \gg a$, giving a corresponding ΔE which is less than V_0. The corresponding odd parity solutions are left to the problems. Using the graphical solutions, it is easy to show that the number of bound states in the well is equal to the integer value of $(1 + \beta/\pi)$.

I can estimate the energy E^+ of the bound state in the limit of a weakly binding well, $\beta \ll 1$. I define

$$z = \sqrt{-\frac{2mE^+}{\hbar^2}}a > 0, \tag{6.90}$$

such that

$$\beta^2 = \left(y^+\right)^2 + z^2. \tag{6.91}$$

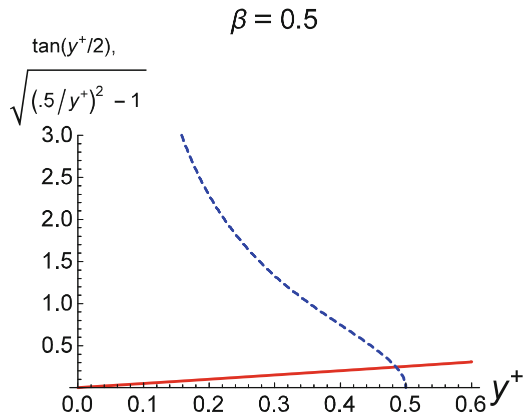

Fig. 6.13 Graphical solution of Eq. (6.88) for $\beta = 0.5$. The blue dashed curve is $\sqrt{(\beta/y^+)^2 - 1}$ and the red solid curve is $\tan\left(y^+/2\right)$

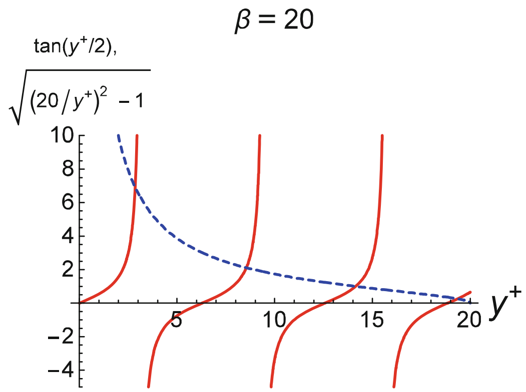

Fig. 6.14 Graphical solution of Eq. (6.88) for $\beta = 20$. The blue dashed curve is $\sqrt{(\beta/y^+)^2 - 1}$ and the red solid curve is $\tan\left(y^+/2\right)$

Setting

$$y^+ = \beta - \epsilon \tag{6.92}$$

and assuming that $\epsilon \ll \beta$ and $\beta \ll 1$, I can approximate Eq. (6.88) as

$$\tan\left(\frac{\beta}{2}\right) \approx \frac{\beta}{2} = \sqrt{\frac{\beta^2}{(\beta-\epsilon)^2} - 1} \approx \sqrt{\frac{2\epsilon}{\beta}} \tag{6.93}$$

or

$$\epsilon \approx \frac{\beta^3}{8}. \tag{6.94}$$

This result, in turn, implies that

$$z^2 = \beta^2 - \left(y^+\right)^2 = \beta^2 - (\beta - \epsilon)^2 \approx 2\epsilon\beta = \beta^4/4 \tag{6.95}$$

or

$$E = -\frac{\hbar^2 z^2}{2ma^2} = -\frac{\hbar^2 \beta^4}{8ma^2} = -\frac{\beta^2}{4} V_0. \tag{6.96}$$

Even if $\beta \ll 1$, there is always a bound state having an energy whose absolute value is much less than the well depth.[4]

In the opposite limit of a very deep well, that is, when $V_0 \to \infty$ and $E' = (E + V_0) \ll V_0$, I should recover the eigenfunctions and eigenenergies of the infinite potential well. In the limit that $V_0 \to \infty$ and $(E + V_0) \ll V_0$, Eqs. (6.88) and (6.89) reduce to

$$\tan\left(\frac{k_E'^{+} a}{2}\right) = \infty, \tag{6.97a}$$

$$\tan\left(\frac{k_E'^{-} a}{2}\right) = 0. \tag{6.97b}$$

The first condition is satisfied if

$$k_E'^{+} a = (2n + 1)\,\pi; \quad n = 0, 1, \ldots \tag{6.98}$$

and the second if

$$k_E'^{-} a = 2n\pi; \quad n = 1, 2, \ldots \tag{6.99}$$

[4]Equation (6.96) can be written as

$$E = -\left(m/2\hbar^2\right) V_0^2 a^2 = -\left(m/2\hbar^2\right) \left[\int_{-\infty}^{\infty} V(x) dx\right]^2.$$

This is a general result for "weak" potential wells having arbitrary shape—see L. D Landau and E. M. Lifshitz, *Quantum Mechanics*, *Non-Relativistic Theory* (Pergamon Press, London, 1958), pp. 155–156.

which, taken together, yield

$$k'_E a = n\pi; \qquad n = 1, 2, 3, \ldots, \tag{6.100}$$

where

$$k'_E = \frac{\sqrt{2m\left(E + V_0\right)}}{\hbar} = \frac{\sqrt{2mE'}}{\hbar}. \tag{6.101}$$

Equation (6.100) is recognized as the equation for the energy levels in an infinite square well. Similarly, the eigenfunctions go over to

$$\psi^+_{II}(x) = A^+ \cos\left(k'^+_E x\right); \tag{6.102}$$

$$\psi^-_{II}(x) = A^- \sin\left(k'^-_E x\right), \tag{6.103}$$

which are the corresponding eigenfunctions.

6.3.2.2 $E > 0$

Since I am interested in transmission and reflection coefficients, I consider only the solution corresponding to a wave incident from the left. The mathematics can be simplified somewhat if I now take the well located between 0 and a. Although the potential no longer commutes with the parity operator with this choice of origin, the solution of interest does not have definite parity in any event since I am considering a wave incident from the left. The eigenfunctions are

$$\psi_E(x) = \begin{cases} Ae^{ik_E x} + Be^{-ik_E x} & x < 0 \\ Ce^{ik'_E x} + De^{-ik'_E x} & 0 < x < a \\ Fe^{ik_E x} & x > a \end{cases} \tag{6.104}$$

with

$$k_E = \frac{\sqrt{2mE}}{\hbar}; \tag{6.105a}$$

$$k'_E = \frac{\sqrt{2m\left(E + V_0\right)}}{\hbar}. \tag{6.105b}$$

I now equate the wave functions in the various regions and their derivatives at both $x = 0$ and $x = a$. The appropriate equations are

$$A + B = C + D; \tag{6.106a}$$

$$k_E\left(A - B\right) = k'_E\left(C - D\right); \tag{6.106b}$$

$$Ce^{ik'_E a} + De^{-ik'_E a} = Fe^{ik_E a}; \tag{6.106c}$$

$$k'_E \left(Ce^{ik'_E a} - De^{-ik'_E a} \right) = k_E Fe^{ik_E a}. \tag{6.106d}$$

From these four equations I can calculate B/A, C/A, D/A, and F/A by setting the determinant of the coefficients equal to zero. The algebra is a little complicated but the solution can be obtained easily using a symbolic program such as Mathematica. Explicitly, you can show that the amplitude reflection and transmission coefficients are equal to

$$R = \frac{B}{A} = \frac{i\left(k_E'^2 - k_E^2\right)\sin\left(k'_E a\right)}{2k_E k'_E \cos\left(k'_E a\right) - i\left(k_E'^2 + k_E^2\right)\sin\left(k'_E a\right)}; \tag{6.107a}$$

$$T = \frac{F}{A} = \frac{2k_E k'_E e^{-ik_E a}}{2k_E k'_E \cos\left(k'_E a\right) - i\left(k_E'^2 + k_E^2\right)\sin\left(k'_E a\right)}. \tag{6.107b}$$

The solution for the intensity transmission coefficient can be written as

$$\mathcal{T} = \frac{J_t}{J_i} = \frac{k_E}{k_E}\left|T\right|^2 = \frac{1}{\cos^2\left(k'_E a\right) + \frac{\epsilon'^2}{4}\sin^2\left(k'_E a\right)} \tag{6.108}$$

and for the intensity reflection coefficient as

$$\mathcal{R} = -\frac{J_r}{J_i} = \frac{k_E}{k_E}\left|R\right|^2 = 1 - \mathcal{T}, \tag{6.109}$$

where

$$\epsilon' = \frac{k_E}{k'_E} + \frac{k'_E}{k_E} = \frac{k_E^2 + k_E'^2}{k_E k'_E} = \frac{2E + V_0}{\sqrt{E}\sqrt{E + V_0}}. \tag{6.110}$$

The intensity transmission coefficient can be written in an alternative way as

$$\mathcal{T} = \frac{1}{1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\left(k'_E a\right)}. \tag{6.111}$$

In the limit that $E \gg V_0$, $\mathcal{T} \sim 1$, as expected, since the energy is much higher than the well depth (recall that, classically, $\mathcal{T} = 1$ for *any* energy $E > 0$). On the other hand, it is not so clear as to what to expect when $E \to 0$, since this corresponds to the quantum regime (de Broglie wavelength greater than well size a). From Eq. (6.111), you see that the transmission goes to zero as $E \to 0$, *unless* $k'_E a = m\pi$, for integer m. That is, there is a *resonance* (sharp increase) in transmission for low energy scattering if $k'_E a \approx \beta = m\pi$. This corresponds approximately to the condition for having a bound state whose energy is very close to zero. For arbitrary energies, there are maxima in transmission whenever $k'_E a = m\pi$. At these points the transmission is equal to unity, but the resonances become broader with increasing energy.

This problem is somewhat analogous to light incident on a thin dielectric film from vacuum if the index of refraction of the film is replaced by

$$n \to n_{\text{eff}} = \sqrt{1 + V_0/E}. \tag{6.112}$$

In optics, when light is incident from vacuum normally on a thin dielectric slab having index of refraction n and thickness d, the reflection and transmission coefficients are

$$\mathcal{R} = 1 - \mathcal{T}; \tag{6.113a}$$

$$\mathcal{T} = \frac{1}{\cos^2(kd) + \frac{\epsilon_n^2}{4}\sin^2(kd)}, \tag{6.113b}$$

where

$$\epsilon_n = n + \frac{1}{n}, \tag{6.114}$$

$$k = nk_0, \tag{6.115}$$

and $k_0 = 2\pi/\lambda_0$ is the free-space propagation constant. The maxima in transmission occur when $kd = m\pi$ or $2d = m\lambda_n = m\lambda_0/n$; that is, when twice the thickness is an integral number of wavelengths in the medium. These are the same resonances that occur in the quantum problem; however, in the quantum problem, the effective index depends significantly on the energy while the index of refraction in the optical problem is approximately constant for a wide range of wavelengths. Details are left to the problems.

If I construct an initial wave packet and send it in from the left, the actual dynamics depends *critically* on the width of the packet. The reflection and transmission coefficients are derived for a *monoenergetic* wave. The range of energies ΔE in the packet must be sufficiently small to satisfy $\Delta E\tau/\hbar \ll 1$, where τ is the time it takes for the packet to be scattered (including bounces back and forth between $x = 0$ and $x = a$) if one is to find transmission and reflection coefficients given by Eqs. (6.108) and (6.109). For example, a wave packet having spatial width less than a could never have a transmission resonance at low energy—it would be totally reflected at the $x = 0$ discontinuity in the potential. Scattering of wave packets in one dimension is discussed in Chap. 17.

The analogy between the quantum and radiation problems is useful only when considering the reflection and transmission coefficients associated with nearly monoenergetic wave packets and nearly monochromatic radiation pulses. The analogy breaks down for wave packets or radiation pulses whose spatial extents are much smaller than the scattering region. For example, you can see from Eq. (6.112)

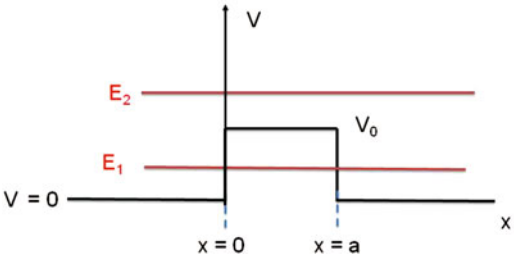

Fig. 6.15 Potential barrier

that a potential well corresponds to an index of refraction $n_{\mathrm{eff}} > 1$. A narrow wave packet would speed up as it passes through the potential region, whereas an optical pulse would propagate at a slower speed in a dielectric corresponding to this potential well.

6.3.3 Potential Barrier

Now I turn my attention to the barrier potential shown in Fig. 6.15 for which

$$V(x) = \begin{cases} V_0 > 0 & 0 < x < a \\ 0 & \text{otherwise} \end{cases}. \tag{6.116}$$

I consider only $E < V_0$. For $E > V_0$, the results of the square well with $E > 0$ can be taken over directly by replacing $-V_0$ with V_0 in Eqs. (6.111) and (6.105b). In the classical problem, a particle is always reflected by the barrier when $E < V_0$. In the quantum-mechanical problem, you will see that the particle can *tunnel* through the barrier. The eigenenergies are continuous and there is a two-fold degeneracy.

As in the case of the potential well, I consider only the eigenfunction corresponding to a wave incident from the left, namely

$$\psi_E(x) = \begin{cases} Ae^{ik_E x} + Be^{-ik_E x} & x < 0 \\ Ce^{\kappa_E x} + De^{-\kappa_E x} & 0 < x < a \\ Fe^{ik_E x} & x > a \end{cases}, \tag{6.117}$$

where

$$k_E = \frac{\sqrt{2mE}}{\hbar} > 0; \tag{6.118}$$

$$\kappa_E = \frac{\sqrt{2m(V_0 - E)}}{\hbar} > 0. \tag{6.119}$$

I should now equate the wave functions in the various regions and their derivatives at both at $x = 0$ and $x = a$. It is not necessary to do so, however, since a comparison of Eqs. (6.104) and (6.117) shows they are identical if I replace ik'_E by κ_E or, equivalently, V_0 by $-V_0$ in Eqs. (6.104). With this replacement, $\sin^2\left(k'_E a\right) \rightarrow -\sinh^2(\kappa_E a)$ and Eq. (6.111) goes over into

$$\mathcal{T} = \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)}\sinh^2(\kappa_E a)}. \tag{6.120}$$

As $E \rightarrow V_0$ ($\kappa_E a \ll 1$), the energy approaches the barrier height and you might expect that significant transmission is possible. In this limit,

$$\mathcal{T} \sim \frac{1}{1 + \frac{V_0^2\kappa_E^2 a^2}{4V_0(V_0-E)}} = \frac{1}{1 + \frac{\beta^2}{4}}, \tag{6.121}$$

where β is defined as in Eq. (6.85). You see that $\mathcal{T} \sim 1$ only if the dimensionless barrier strength β is much less than unity. Note that Eq. (6.121) agrees with Eq. (6.111) when V_0 is replaced by $-V_0$ in that equation and the limit $E \rightarrow V_0$ is taken. In other words, the solutions for $E < V_0$ and $E > V_0$ match each other in the limit that $E \rightarrow V_0$, as you would expect.

On the other hand, for $\kappa_E a \gg 1$,

$$\mathcal{T} \sim \frac{16(V_0 - E)E}{V_0^2} e^{-2\kappa_E a}, \tag{6.122}$$

which represents *tunneling* through the barrier. [If you play tennis, you are familiar with tunneling—you swear you hit the ball, but it appears to have tunneled through your racket. Unfortunately this argument does not hold water since the tunneling probability is negligibly small)]. In the limit that $\hbar \rightarrow 0$, $\kappa_E \sim \infty$, the de Broglie wavelength goes to zero, and there is no tunneling. Tunneling can occur in optics if two prisms are separated by a small amount, as was originally discovered by Newton. Light that would normally be totally internally reflected by the first prism can tunnel into the second prism if the separation between the prisms is less than or on the order light's wavelength. Tunneling is a wave phenomenon.

6.4 Delta Function Potential Well and Barrier

The limit of a *delta function potential*,

$$V(x) = \pm V_0 a\delta(x), \tag{6.123}$$

can be approximated if I let the potential well or barrier width a go to zero while its amplitude V_0 goes to infinity, keeping the product $V_0 a$ constant. In Eq. (6.123) both V_0 and a are positive; the plus sign corresponds to a barrier and the minus sign to a potential well. From the nature of the solutions of the potential barrier or well problems, it follows that the wave function is continuous at the position of the delta function potential. On the other hand, the derivative of the wave function undergoes a jump. To see this, I start from the Schrödinger equation

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}\left[E - V(x)\right]\psi(x) \tag{6.124}$$

and integrate about $x = 0$ to obtain

$$\begin{aligned} \left.\frac{d\psi(x)}{dx}\right|_{x=\epsilon} - \left.\frac{d\psi(x)}{dx}\right|_{x=-\epsilon} &= -\lim_{\epsilon\to 0}\frac{2m}{\hbar^2}\int_{-\epsilon}^{\epsilon}\left[E - V(x)\right]\psi(x)dx \\ &= -\lim_{\epsilon\to 0}\frac{2m\psi(0)}{\hbar^2}\int_{-\epsilon}^{\epsilon}\left[E - V(x)\right]dx \\ &= \pm\frac{2mV_0a\psi(0)}{\hbar^2}. \end{aligned} \tag{6.125}$$

The derivative of the wave function undergoes a point jump discontinuity at the position of the delta function potential.

6.4.1 Square Well with $E < 0$

As $a \to 0$ in the square well problem, the dimensionless strength parameter $\beta^2 = 2mV_0a^2/\hbar^2 \to 0$, since V_0a goes to a constant and $a \to 0$. If $\beta^2 \to 0$, the only bound state solution is the lowest energy, even parity solution. The energy is determined from Eq. (6.96),

$$E = -\frac{\hbar^2\beta^4}{8ma^2} = -\frac{mV_0^2a^2}{2\hbar^2}. \tag{6.126}$$

Now let's solve the problem directly. With $\kappa_E = \sqrt{-2mE/\hbar^2}$, the eigenfunction of the bound state can be taken as

$$\psi_E(x) = \begin{cases} Be^{\kappa_E x} & x < 0 \\ Be^{-\kappa_E x} & x > 0 \end{cases}, \tag{6.127}$$

which satisfies continuity of the wave function at $x = 0$. Using Eq. (6.125), I find

$$\begin{aligned} \left.\frac{d\psi(x)}{dx}\right|_{x=\epsilon} - \left.\frac{d\psi(x)}{dx}\right|_{x=-\epsilon} &= -2B\kappa_E = -2B\sqrt{-\frac{2mE}{\hbar^2}} \\ &= -\frac{2mV_0a\psi(0)}{\hbar^2} = -\frac{2mV_0aB}{\hbar^2}. \end{aligned} \tag{6.128}$$

Therefore,

$$-\frac{2mE}{\hbar^2}=\left(\frac{mV_0a}{\hbar^2}\right)^2; \tag{6.129}$$

$$E=-\frac{mV_0^2a^2}{2\hbar^2}, \tag{6.130}$$

in agreement with Eq. (6.126).

6.4.2 Barrier with $E > 0$

From Eq. (6.120), with $V_0 \gg E$ and $\kappa_E a \approx \beta \rightarrow 0$,

$$\mathcal{T}=\frac{1}{1+\frac{V_0^2}{4E(V_0-E)}\sinh^2(\kappa_E a)}\simeq\frac{1}{1+\frac{V_0\beta^2}{4E}}=\frac{1}{1+\frac{mV_0^2a^2}{2\hbar^2E}}. \tag{6.131}$$

To solve the problem directly, I take

$$\psi_E(x)=\begin{cases}Ae^{ik_Ex}+Be^{-ik_Ex}; & x<0\\ Fe^{ik_Ex} & x>0\end{cases}, \tag{6.132}$$

where $k_E=\sqrt{2mE/\hbar^2}$. The wave function is continuous at $x=0$ and its derivative undergoes a jump discontinuity,

$$A+B=F; \tag{6.133}$$

$$\left.\frac{d\psi(x)}{dx}\right|_{x=\epsilon}-\left.\frac{d\psi(x)}{dx}\right|_{x=-\epsilon}=ik_E(F-A+B)$$
$$=\frac{2mV_0a\psi(0)}{\hbar^2}=\frac{2mV_0aF}{\hbar^2}, \tag{6.134}$$

which can be rewritten as

$$-\frac{B}{A}+\frac{F}{A}=1; \tag{6.135}$$

$$\frac{B}{A}+\frac{F}{A}\left(1+\frac{2imV_0a}{k_E\hbar^2}\right)=1. \tag{6.136}$$

Solving for the transmission coefficient, I find

$$\mathcal{T}=\left|\frac{F}{A}\right|^2=\frac{4}{\left|2+\frac{2imV_0a}{k_E\hbar^2}\right|^2}=\frac{1}{1+\frac{mV_0^2a^2}{2\hbar^2E}}=\frac{1}{1+\left(\frac{\beta^2}{2k_Ea}\right)^2}, \tag{6.137}$$

in agreement with Eq. (6.131). In the limit $\beta^2 V_0/4E = mV_0^2a^2/2\hbar^2E \gg 1$, $\mathcal{T} \sim 0$, which is the *strong barrier limit*. On the other hand, for $\beta^2 V_0/4E \ll 1$, the transmission goes to unity. If you consider the problem of transmission for a negative delta function potential, the transmission coefficient is unchanged, since $\mathcal{T}$ depends only on V_0^2.

6.5 Summary

I have examined a number of prototypical one-dimensional problems in quantum mechanics involving piecewise constant potentials. In all these problems, I was able to solve the Schrödinger equation in a number of distinct regions and piece together the solutions using the continuity of the wave function and its derivative. In considering the motion of particles in potentials that change abruptly at a given point, we always encounter wave-like properties of the particles since the potential changes in a distance small compared with the de Broglie wavelength of the particle. In the limit that $\hbar \to 0$ in such problems, we recover the geometrical or ray optics limit of optics for light incident on a dielectric interface. Processes such as transmission and reflection resonances, as well as tunneling, have optical analogues.

6.6 Appendix: Periodic Potentials

To arrive at the band structure of solids, one often models the problem of electrons interacting with atomic sites in a crystal by considering the electrons to move in a periodic potential having period d. If periodic boundary conditions are imposed, it is possible to find eigenfunctions $\psi_E(x)$ that satisfy Bloch's theorem,

$$\psi_E(x) = e^{i\alpha x/d} u_E(x), \tag{6.138}$$

where $u_E(x)$ is a periodic function having period d and α is the *Bloch phase*. Both α and $u_E(x)$ are functions of the energy E and the detailed nature of the potential. It is possible to relate the Bloch states to the transmission resonances that occur when matter waves are incident on an equally spaced array of identical potential barriers.[5] The problem can then be mapped onto one involving periodic boundary conditions by imposing the requirement that the wave function at the entrance of the array be equal to the wave function at the exit. I will consider only the problem of the transmission resonances in detail, but then make a connection with the Bloch states.

[5]For a more detailed discussion with references to earlier work, see P. R. Berman, *Transmission resonances and Bloch states from a periodic array of delta function potentials,* American Journal of Physics, **81**, 190–201 (2013).

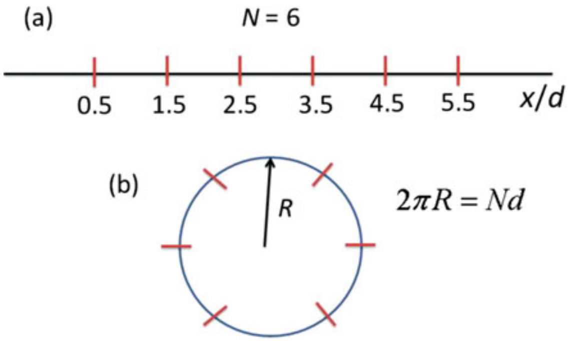

Fig. 6.16 (**a**) A finite array of delta function potentials on a line. (**b**) A periodic array of delta function potentials on a ring

To simplify the problem, I take the potential as

$$V(x) = V_0 a \sum_{j=1}^{N} \delta\left(x - \frac{2j-1}{2}d\right), \tag{6.139}$$

where V_0 and a are positive constants. The array has period d in the interval from $x = 0$ to $x = Nd$ with a delta function at the middle of each period [see Fig. 6.16a]. Periodic potentials with rectangular barriers constitute the so-called *Kronig-Penney model*. The wave function is taken as

$$\psi(x) = \begin{cases} A_0 e^{izx} + B_0 e^{-izx} = e^{izx} + R_N e^{-izx} & -\infty < x < 1/2 \\ A_n e^{iz(x-n)} + B_n e^{-iz(x-n)} & \left(n - \frac{1}{2}\right) < x < \left(n + \frac{1}{2}\right) \\ A_N e^{iz(x-N)} + B_N e^{-iz(x-N)} = T_N e^{iz(x-N)} & x > \left(N - \frac{1}{2}\right) \end{cases}, \tag{6.140}$$

where $z = kd$, $k = \sqrt{2mE}/\hbar$, and $1 \leq n \leq N-1$. The quantity x has been redefined to be dimensionless, measured in units of the period d, and I have set $A_0 = 1$ and $B_0 = R_N$. With this choice, the quantities R_N and T_N are the reflection and transmission *amplitudes* for an N-period array, for a wave incident from the left.

By matching the wave function and its (discontinuous) derivative at $x = \left(n - \frac{1}{2}\right)$ using Eq. (6.140), I find

$$\begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix} = \mathbf{M} \begin{pmatrix} A_n \\ B_n \end{pmatrix}, \tag{6.141}$$

where

$$\mathbf{M} = \begin{pmatrix} we^{-iz} & y \\ y^* & e^{iz}w^* \end{pmatrix}, \tag{6.142}$$

and

$$w = (1 + i\chi)\,; \quad y = i\chi, \tag{6.143}$$

with

$$\chi = z_0/z, \tag{6.144a}$$

$$z = kd, \tag{6.144b}$$

$$z_0 = \frac{mV_0 a}{\hbar^2} d. \tag{6.144c}$$

The matrix **M** is a *transfer matrix*. Had I considered potentials other than a delta function potential, the form of **M** would remain the same, but the values of w and y would change, subject to the constraint

$$|w|^2 - |y|^2 = 1, \tag{6.145}$$

provided by unitarity. Many of the equations are left in terms of w and y, but all calculations are performed for delta function potentials.

The transmission coefficient can now be calculated by writing

$$\begin{pmatrix} 1 \\ R_N \end{pmatrix} = \mathbf{M}_N \begin{pmatrix} T_N \\ 0 \end{pmatrix}, \tag{6.146}$$

with

$$\mathbf{M}_N = \mathbf{M}^N. \tag{6.147}$$

Thus, it is clear that

$$T_N = 1/\left(M_N\right)_{11}\,; \tag{6.148a}$$

$$R_N = \left(M_N\right)_{21} T_N = \left(M_N\right)_{21} / \left(M_N\right)_{11}. \tag{6.148b}$$

The amazing thing is that $\mathbf{M}_N$ can be calculated analytically for any N. It is possible to write the result for $\mathbf{M}_N$, T_N, and R_N in the compact form

$$\mathbf{M}_N = \frac{\mathbf{M}\sin(N\phi) - \mathbf{1}\sin[(N-1)\phi]}{\sin\phi}, \tag{6.149a}$$

$$\frac{1}{T_N} = \frac{M_{11}\sin(N\phi) - \sin[(N-1)\phi]}{\sin\phi} = \frac{we^{-iz}\sin(N\phi) - \sin[(N-1)\phi]}{\sin\phi}, \tag{6.149b}$$

$$R_N = \frac{M_{21}}{M_{11}}\left[1+\frac{\sin\left[(N-1)\,\phi\right]}{\sin\phi}T_N\right]$$
$$= \frac{y^* e^{iz}}{w}\left[1+\frac{\sin\left[(N-1)\,\phi\right]}{\sin\phi}T_N\right], \tag{6.149c}$$

where ϕ is defined by

$$\cos\phi = \mathrm{Re}\,(M_{11}) = \mathrm{Re}\,(1/T_1) = \mathrm{Re}\,(w\cos z) + \mathrm{Im}\,(w\sin z)\,, \tag{6.150}$$

and **1** is the 2×2 identity matrix. This completes the solution to the problem.

It is not difficult to calculate the energies for which the transmitted intensity is equal to unity using Eq. (6.149b). I need to find values $\phi = \phi_T$ for which

$$\frac{1}{T_N} = \frac{M_{11}\sin\left(N\phi_T\right) - \sin\left[(N-1)\,\phi_T\right]}{\sin\phi_T} = \pm 1. \tag{6.151}$$

For arbitrary M_{11} the solution is obtained by setting

$$\frac{\sin\left(N\phi_T\right)}{\sin\phi_T} = 0, \tag{6.152a}$$

$$-\frac{\sin\left[(N-1)\,\phi_T\right]}{\sin\phi_T} = \cos(N\phi_T) = \pm 1. \tag{6.152b}$$

These equations are satisfied if

$$\phi_T = q\pi/N; \qquad q = 1, 2, \ldots, N-1. \tag{6.153}$$

Note that q cannot be equal to zero or N since $\phi_T = 0$ and π are *not* solutions of Eq. (6.151). For each value of q, there is an infinite number of solutions of Eq. (6.150) for $z = kd$, with successive solutions corresponding to different *energy bands*. Since q can take on $N-1$ distinct values, there are $N-1$ transmission resonances in each band. The transmission amplitude at each *transmission resonance* is $T_N = (-1)^q$.

The transmission coefficient $\mathcal{T}_N = |T_N|^2$ is shown in Fig. 6.17 for $N = 10$ and $z_0 = 5$ as a function of $z/\pi = kd/\pi$. You can see that the transmission peaks are contained in bands which (almost) go over into the band structure of crystals. The upper band edge of the mth band is close, but not equal to $z = m\pi$. A blow-up of the first band is shown in Fig. 6.18 and the real part of the transmission amplitude for this band is shown in Fig. 6.19.

In general, there are $(N-1)$ transmission peaks contained in each band. Of the $N-1$ resonances, there are $(N-2)/2$ values where $T_N = 1$ when N is even and $(N-1)/2$ values where $T_N = 1$ when N is odd. The other resonances correspond to $T_N = -1$. I will return to this shortly.

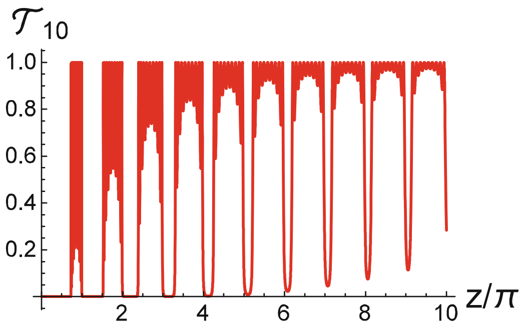

Fig. 6.17 Intensity transmission coefficient for a periodic array of 10 delta functions with $z_0 = 5$

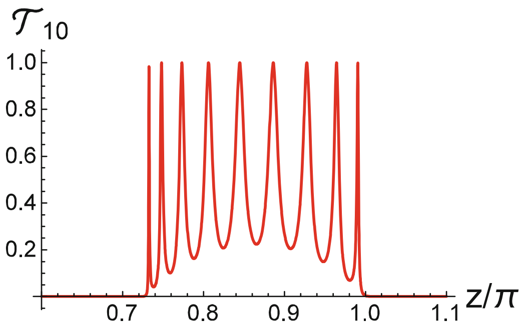

Fig. 6.18 Blow-up of the first "band" of the intensity transmission coefficient for a periodic array of 10 delta functions with $z_0 = 5$. There are $(N - 1) = 9$ transmission resonances in each band

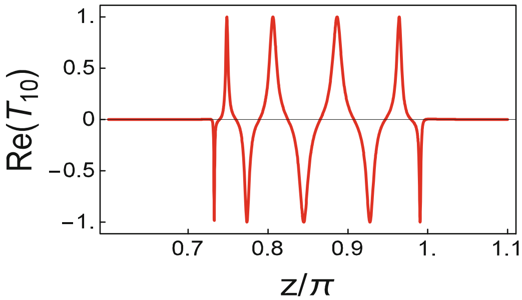

Fig. 6.19 Real part of the transmission *amplitude* in the first "band" of a periodic array of 10 delta functions with $z_0 = 5$. There are four resonances with $T = 1$ and five with $T = -1$

The net result is that, in the low energy bands where $\chi = z_0/m\pi \gg 1$, the transmission resonances are resolved and correspond to quasi-bound states of the "lattice." The quasi-resonances are confined to these energy bands and the width of the mth band, with upper band edge at $z \approx m\pi$, is of order $\Delta z = \Delta kd \sim 2m\pi/z_0$ for delta function potentials. On the other hand, for high energies, $\chi = z_0/m\pi \ll 1$, the transmission resonances are not resolved and form a series of bands with narrow gaps between the bands, having a gap width $\Delta z = \Delta kd \sim 2z_0/m\pi$ for delta function potentials. In these high energy bands (not yet seen in Fig. 6.17) $\mathcal{T}_N \approx 1$. The high energy bands correspond to quasi-free particle states that can exist at these energies.

6.6.1 Bloch States

The Bloch theory of a crystal assumes a *periodic potential* in *all* space. Of course, no crystal exists in all space, so what is usually done is to imagine the periodic potential on a ring, that is, N identical delta function potentials, periodically placed on a ring [see Fig. 6.16b]. I can map the ring, having radius R, onto a line of length $L = 2\pi R = Nd$ with $\psi(x = 0) = \psi(x = L/d)$, and

$$\theta = 2\pi x/N. \tag{6.154}$$

The ring radius R grows with increasing N for fixed d.

It can be shown that the Bloch energies correspond to a *subset* of the solutions associated with Eq. (6.153), containing those values for which $T_N = 1$, but *not* those for $T_N = -1$. The wave functions with $T_N = -1$ are out of phase by π when they return to the same physical point. This implies that there are approximately *half* as many Bloch state energies as transmission energies, but each of these Bloch states is two-fold degenerate, since waves can move either clockwise or counterclockwise. Moreover, there are additional Bloch energies that occur that are absent in the transmission resonances, namely values of ϕ which are equal to zero or π.

As a consequence, the energy "bands," each contain $(N + 2)/2$ discrete energy levels for N even and $(N + 1)/2$ discrete energy levels for N odd. The discrete energies correspond to the transmission resonances for which $T_N = 1$, *plus* an energy eigenfunction for $\phi = 0$ and, if N is even, an additional one for $\phi = \pi$. Each state is two-fold degenerate, *except* for those corresponding to $\phi = 0$ or π. Thus there are $2[(N + 2)/2 - 2] + 2 = N$ states for N even and $2[(N + 1)/2 - 1] + 1 = N$ states for N odd. Each band contains exactly N states. Note that as $N \to \infty$, the number of states in each band goes to infinity but the states remain discrete. Despite the fact that these states remain discrete, the resulting structure is referred to as the (continuous) band structure of solids.

6.7 Problems

1. Show that solutions of

$$\frac{d^2 f}{dx^2} = -k^2 f$$

are $e^{\pm ikx}$ and solutions of

$$\frac{d^2f}{dx^2} = k^2 f$$

are $e^{\pm kx}$.

2. Suppose you are given a constant potential V_0 in some region of space in a one-dimensional problem. For energies $E > V_0$ (classically allowed region), prove that possible solutions of the Schrödinger equation are $e^{ik'x}$, $e^{-ik'x}$, $\cos(k'x)$, $\sin(k'x)$, provided $k' = \sqrt{2m(E - V_0)/\hbar^2}$. For energies $E < V_0$ (classically forbidden region), prove that possible solutions of the Schrödinger equation are $e^{\kappa x}$, $e^{-\kappa x}$, $\cosh(\kappa x)$, $\sinh(\kappa x)$, provided $\kappa = \sqrt{2m(V_0 - E)/\hbar^2}$. In each case, why is the eigenfunction in that region a linear combination of at most two of the four solutions shown? What determines which linear combination and how many independent solutions are needed?

3. What is the difference in energy between the two lowest energy states of a 1.0 g particle moving in a 1.0 cm infinite square well potential? What does this tell you about measuring the energy spacing of the quantized states of a macroscopic particle?

4–5. At $t = 0$, the wave function for a particle of mass m in an infinite one-dimensional potential well located between $x = 0$ and $x = L$ is equal to

$$\psi(x,0) = \begin{cases} e^{-(x-L/2)^2/2x_0{}^2} & 0 < x < L \\ 0 & \text{otherwise} \end{cases},$$

which can be expanded as

$$\psi(x,0) = \begin{cases} \sqrt{2/L}\sum_{n=1}^{\infty} a_n \sin(n\pi x/L) & 0 < x < L \\ 0 & \text{otherwise} \end{cases},$$

where $x_0 << L$ [note that $\psi(x,0)$ is not normalized, but it is not important for this problem—it just gives an overall scaling factor to the a_n's]. In practice, you must cut off the sum at some value $n = n_{\text{max}}$. Without formally solving the problem, estimate the value of n_{max} needed to provide a good approximation to $\psi(x,0)$. Now show that your estimate is reasonable by taking $L = 100$, $x_0 = 1$, and numerically integrating the appropriate equation to obtain the a_ns to find the maximum n that contributes significantly.

6–7. The k-state probability distribution for the eigenfunctions of the infinite square well having width L is given by [see Eq. (6.28)]

$$|\phi_n(k)|^2 = \frac{\pi L n^2 \left|1 - (-1)^n e^{-ikL}\right|^2}{\left[(kL)^2 - (n\pi)^2\right]^2}.$$

First, prove that the height of the lobes centered at $k = \pm n\pi/L$ in the limit that $n \gg 1$ is equal to $L/4\pi$. Next show that the half width at half maximum of each lobe is approximately equal to $2.79/L$ when $n \gg 1$. [Hint: Set $k = n\pi/L + \epsilon$ with $\epsilon \ll n\pi/L$ and solve the equation

$$|\phi_n(n\pi/L + \epsilon)|^2 = L/8\pi.$$

Note you *cannot* assume that $e^{iL\epsilon} \approx 1 + iL\epsilon$ since it will turn out that ϵ is of order $1/L$.]

8. For the potential step problem with energy $E > V_0$, consider the eigenfunction

$$\psi_E^R(x) = \begin{cases} \psi_{IE}^R(x) & x < 0 \\ \psi_{IIE}^R(x) & x > 0 \end{cases},$$

where

$$\psi_{IE}^R(x) = C_R e^{-ik_E x};$$
$$\psi_{IIE}^R(x) = A_R e^{-ik'_E x} + B_R e^{ik'_E x},$$

corresponds to a wave incident from the right. Calculate the amplitude reflection and transmission coefficients, R and T, and show that they can be obtained from those for the left incident wave by interchanging k_E and k'_E. Prove that the intensity reflection and transmission coefficients, $\mathcal{R}$ and $\mathcal{T}$, are unchanged. The quantities k_E and k'_E are defined in Eqs. (6.47) and (6.62), respectively.

9. One of the eigenfunctions for the step potential problem with energy $E > V_0$ is

$$\psi_{k_E}^L(x) = \begin{cases} \left(e^{ik_E x} + \frac{k_E - k'_E}{k_E + k'_E} e^{-ik_E x}\right) & x < 0 \\ \left(\frac{2k_E}{k_E + k'_E}\right) e^{ik'_E x} & x > 0 \end{cases} \qquad k_E > 0.$$

Calculate the probability current density of the entire wave function (do not break up the $x < 0$ part into incident and reflected waves) for $x < 0$ and $x > 0$ and show that the two results agree at $x = 0$. In fact, show that the current density is constant in all space. The quantities k_E and k'_E are defined in Eqs. (6.47) and (6.62), respectively.

10. The eigenfunctions for the step potential with energy $E < V_0$ is

$$\psi_{k_E}^L(x) = \begin{cases} \left(e^{ik_E x} + \frac{k_E - i\kappa_E}{k_E + i\kappa_E} e^{-ik_E x}\right) & x < 0 \\ \left(\frac{2k_E}{k_E + i\kappa_E}\right) e^{-\kappa_E x} & x > 0 \end{cases} \qquad k_E > 0.$$

Calculate the probability current density of the entire wave function and show that it vanishes in all space. The quantities k_E and κ_E are defined in Eqs. (6.47) and (6.50), respectively.

11. Obtain a graphical solution for the odd parity eigenenergies of the potential well problem. Find the minimum value of $\beta = \sqrt{\frac{2mV_0}{\hbar^2}a^2}$ needed to support an odd parity bound state.

12. Suppose a potential well having depth V_0 and width b is located inside of an *infinite* potential well having width $a > b$. Use a simple argument based on the uncertainty principle to derive an approximate condition for the existence of a bound state having $E < 0$. How does this problem differ from the one studied in the text, in which it was shown that a bound state always exists?

13–14. Now solve Problem 6.12 formally. Take both the finite well and infinite well centered at $x = 0$, such that the Hamiltonian commutes with the parity operator. Find the condition on V_0, b, and a, that will guarantee at least one bound state for $E < 0$. Show that in the limit that $a \rightarrow \infty$, there is always a bound state. Hint: What parity will the lowest energy state have? Choose a wave function that automatically satisfies the boundary condition at $x = a/2$.

15–18. In optics, when light is incident normally on a thin dielectric slab having index of refraction n and thickness d, the reflection and transmission coefficients are

$$\mathcal{R} = 1 - \mathcal{T};$$
$$\mathcal{T} = \frac{1}{\cos^2(kd) + \frac{\epsilon_n^2}{4}\sin^2(kd)},$$

where

$$\epsilon_n = n + \frac{1}{n},$$
$$k = nk_0,$$

and $k_0 = 2\pi/\lambda_0$ is the free-space propagation constant. Plot $\mathcal{T}$ as a function of $k_0 d$ for $n = 2$ and $n = 6$. Interpret your plots—that is, explain the positions of the maxima and minima in transmission on the basis of simple principles of optics.

In quantum mechanics, prove that the corresponding reflection and transmission coefficients for scattering of a particle having mass m by a potential barrier having length d and height V_0 are *identical*, provided one sets

$$n \rightarrow n_E = \sqrt{1 - V_0/E};$$
$$k \rightarrow k'_E = n_E k_E = n_E\sqrt{\frac{2mE}{\hbar^2}} = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}.$$

It is assumed that $E > V_0$. The difference from the radiation problem is that as k_E is varied, the index n_E changes as well, whereas k_0 can be changed in the radiation problem without changing the index significantly. Thus it makes sense to define

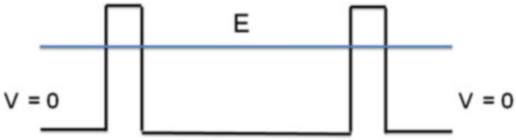

Fig. 6.20 Problem 6.21

$$k'_E d = \theta; \qquad \alpha = E/V_0;$$

$$\theta = \theta_0\sqrt{\left(\frac{E-V_0}{V_0}\right)} = \theta_0\sqrt{\alpha-1};$$

$$\theta_0 = \sqrt{\frac{2mV_0}{\hbar^2}}d;$$

$$\mathcal{T} = \frac{1}{\cos^2\theta + \frac{\epsilon_{nE}^2}{4}\sin^2\theta},$$

so that the only parameters in the problem are θ_0 and $\alpha = E/V_0$. Plot $\mathcal{T}$ as a function of α for $\theta_0 = 10, \alpha = (1,4)$ and $\theta_0 = 100, \alpha = (1, 1.05)$. Qualitatively how do the results differ from the radiation case? Note that with increasing θ_0 you would need better energy resolution in your incident beam to be able see the resonances. That is if you used too wide an energy bin, you could miss some of the resonances.

19. Calculate the transmission coefficient for a potential barrier having a height of 3 eV when a particle having energy 1 eV is incident, assuming the particle mass is 1 g and the barrier width is 1 cm.

20. Calculate the reflection and transmission coefficients for a particle having mass m scattered by the potential $V(x) = V_0 a\delta(x)$, where V_0 and a are positive constants.

21. For the double barrier potential shown in Fig. 6.20 it turns out that there are certain energies where the transmission is 100%, even though the transmission coefficient of *each* barrier is much less than unity. How can that be if it is very difficult for a particle incident from the left to tunnel into the space between the barriers and then tunnel out of the other side?

22. For a particle in an infinite potential well centered at the origin, prove that quantum revivals $[|\psi(x,t)|^2 = |\psi(x,0)|^2]$ occur for times t that are integral multiples of $t_r/8$ if the initial wave function is symmetric about the origin and for times t that are integral multiples of $t_r/4$ if the initial wave function is antisymmetric about the origin, where t_r is given by Eq. (6.44).

23. For a particle in an infinite potential well centered at the origin, prove that

$$|\psi(-x, t_r/2)|^2 = |\psi(x,0)|^2$$

where t_r is given by Eq. (6.44). This result implies that there are quantum revivals at $t = t_r/2$ whenever the absolute square of the initial wave packet is either symmetric or antisymmetric about the origin.

6.7.1 Advanced Problems

1. There are two ways to calculate the expectation values of $\hat{k}^2$ and $\hat{k}^4$ $\left(\hat{k} = \hat{p}/\hbar\right)$ in an eigenstate of the particle in an infinite square well potential. One is to use $|\phi_n(k)|^2$ given in Problem 6.6–7, while the other is to use

$$\hat{k} = \frac{1}{i}\frac{d}{dx}$$

and work with the spatial eigenfunctions. Prove that both methods lead to the same value for $\left\langle \hat{k}^2 \right\rangle$. Now show that the coordinate space method leads to a finite value of $\left\langle \hat{k}^4 \right\rangle$, while the momentum space method yields an infinite result. This problem shows you that some care must be taken when the Fourier transform of the potential is not well defined. The momentum space method gives the correct (infinite) result.[6]

2. Solve Newton's equations of motion (that is, do not simply use energy conservation, solve for the dynamics) for a *classical* particle incident from the left on a potential step in one dimension. Consider both $E < V_0$ and $E > V_0$. Show that you arrive at results consistent with energy conservation. To solve this problem, replace the "step" by a ramp potential

$$V(x) = \lim_{a \to 0^+} \begin{cases} V_0\,(x+a)\,/2a & -a < x < |a| \\ 0 & x \le -a \\ V_0 & x \ge a \end{cases},$$

where $\lim_{a \to 0^+}$ means that a approaches zero from positive values. The slope of the ramp potential is $V_0/2a$ and approaches a potential step as $a \to 0^+$. Use this potential to solve Newton's equation for the position and velocity of the particle and then take the limit that $a \to 0^+$.

[6] See F. E. Cummings, *The particle in a box is not simple*, American Journal of Physics, Volume **45,** pp 158–160 (1977), who looks at the infinite well as the limit of a potential having steep walls. Alberto Rojo of Oakland University sent me an alternative calculation to prove that $\left\langle \hat{k}^4 \right\rangle$ diverges by considering the infinite well as the limit of a finite well whose depth is then allowed to go to infinity.

3. Normalize the wave function

$$\psi_k^L(x) = N \begin{cases} \left(e^{ikx} + \frac{k-d(k)}{k+d(k)} e^{-ikx}\right) & x < 0 \\ \frac{2k}{k+d(k)} e^{id(k)x} & x > 0 \end{cases} \qquad k > 0,$$

where

$$d(k) = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} = \sqrt{k^2 - \frac{2mV_0}{\hbar^2}}.$$

To do this write

$$\psi_k^L(x) = N \lim_{\epsilon \to 0+} \begin{cases} \left(e^{ikx} + \frac{k-d(k)}{k+d(k)} e^{-ikx}\right) e^{\epsilon x/2} & x < 0 \\ \frac{2k}{k+d(k)} e^{id(k)x} e^{-\epsilon x/2} & x > 0 \end{cases} \qquad k > 0,$$

and find N such that

$$\int_{-\infty}^{\infty} dx \left[\psi_{k'}^L(x)\right]^* \psi_k^L(x) = \delta\left(k - k'\right)$$

in the limit that $\epsilon \to 0$ from positive values.

4. Consider a particle having mass m in the potential

$$V(x) = V_0 a \left[\delta(x) + \delta(x-b)\right],$$

where V_0, a, and b are positive constants. Moreover consider the limit $\beta^2/k_E a \gg 1$, where $k_E = \sqrt{2mE}/\hbar$, for which the transmission of a single barrier is small. Write the eigenfunctions as

$$\psi_E(x) = \begin{cases} e^{ik_E x} + Be^{-ik_E x} & x < 0 \\ Ce^{ik_E x} + De^{-ik_E x} & 0 \le x \le b \\ Fe^{ik_E x} & x > b \end{cases}.$$

Plot the transmission coefficient $\mathcal{T} = |F|^2$ as a function of $y = k_E b$ for $\beta' = 8$ and $0 \le y \le 20$ and show that $\mathcal{T} = 1$ when $y \approx q\pi$, for integer q. The quantity β' is defined by

$$\beta'^2 = \frac{2mV_0 ab}{\hbar^2} = \beta^2 \frac{b}{a}.$$

Also plot $|C|^2$ for the same values to show that the wave between the barriers is large compared to that outside the barriers at resonance. Interpret your result in terms of quasibound states between the barriers.

5. A particle having mass m moves in a one-dimensional potential

$$V(x) = \begin{cases} 0 & x < 0 \\ -V_0 < 0 & 0 < x < a \\ V_1 > 0 & x > a \end{cases} .$$

Write the general form of the eigenfunctions for bound states having $E < 0$ that satisfy the boundary conditions as $|x| \sim \infty$. Using the boundary conditions at $x = 0$ and $x = a$ obtain a single equation that could be solved graphically to obtain the eigenenergies. It simplifies the solution if you use sin and cos solutions for $0 < x < a$. Prove that, in the limit of a very weak well, $\beta_0^2 = 2mV_0a^2/\hbar^2 \ll 1$, a bound state exists only if $\beta_1 < \beta_0^2$, where $\beta_1^2 = \frac{2mV_1}{\hbar^2}a^2$.