Chapter 17
Scattering: 1-D

Most of what we know about the structure of matter comes from scattering experiments. When I discuss scattering in 3-D, I will review classical scattering theory, but for the time being, I want to discuss the scattering problem in one-dimension. Scattering is simple in principle—send something in and see what comes out. I will give a detailed analysis of scattering in one-dimension for the step potential shown in Fig. 17.1 and then give a qualitative discussion for other potentials. The step potential can be written as

$$V(x) = V_0 \Theta(x), \tag{17.1}$$

where $\Theta(x)$ is the Heaviside step function which is zero for $x < 0$ and one for $x \geq 0$.

Classically, this is a simple problem. If the energy of a particle incident from the left is less than V_0, it is reflected at the potential step with a change in the sign of its velocity; if the energy is greater than V_0 there is no reflection and the particle is transmitted with reduced energy. However, for a true step potential, the problem is *always* quantum-mechanical in nature since the potential changes over a distance that is small compared to a de Broglie wavelength of the particle. In that case, part of the wave packet is always reflected if $E > V_0$. Of course, a *real* potential can only approximate a step function; quantum mechanics is needed if the potential changes over a distance that is small compared to a de Broglie wavelength of the particle. As you will see, there is an additional quantum effect when the energy is less than the height of the step.

There are two basic approaches to solving a scattering problem. In the *steady-state* approach, it is assumed that some type of steady-state has been reached in which a continuous, mono-energetic beam of particles is incident on the scattering region. You can then identify a current density for both the incident and scattered particles. This is the easiest way to do scattering theory and corresponds to the idealized situation in which there is a single energy in the problem, since the incoming beam is mono-energetic. In effect we deal with a *single* energy

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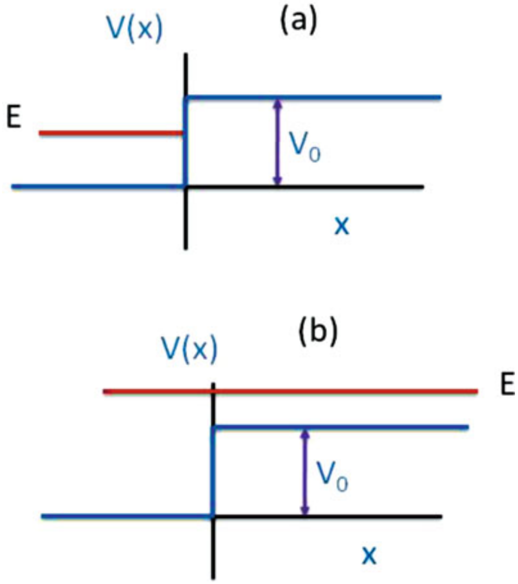

Fig. 17.1 Step potential: (**a**) Energy less than the barrier height. (**b**) Energy greater than the barrier height

eigenstate of the system. The second approach is more difficult mathematically, but more interesting from a physical viewpoint. In this *time-dependent* approach, one sends in a wave packet to the scattering region and looks at the emerging wave packets. Both methods give identical results for the reflection and transmission coefficients when the spatial width of the wave packet is taken to be arbitrarily large (approaching a mono-energetic wave). Scattering is usually a uniquely well-defined problem only in this limit.

Before we start, let me consider the classical scattering problem with one particle a second having energy $E > V_0$ moving towards the step potential from the left with a velocity of one meter per second. The situation is depicted in Fig. 17.2 for successive times differing by one second. As can be seen, the density per unit length *increases* for particles once they are past the barrier, and the speed of each particle *decreases*. However the current density $J = \mathcal{N}v$, where $\mathcal{N}$ is the density per unit length, remains *constant*. The ratio of the transmitted to incident particle current density is a measure of the transmission coefficient, which is unity in the classical case.

Returning to the quantum problem, I proceed as in any problem in quantum mechanics by finding the stationary state eigenfunctions. If $E_k = \hbar^2k^2/2m > V_0$ and m is the mass of the particle, independent (normalized) eigenfunctions for the potential step may be taken as

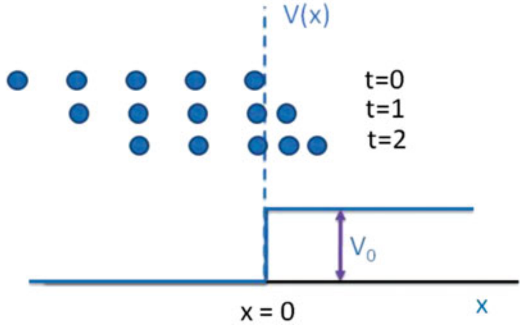

Fig. 17.2 Particles passing the barrier slow down, but their density increases in such a manner that the particle current density remains constant

$$\psi_k^+(x) = \frac{\Theta(k)}{\sqrt{2\pi}} \begin{cases} e^{ikx} + a(k)e^{-ikx} & x < 0 \\ b(k)e^{ik'x} & x \geq 0 \end{cases}; \tag{17.2a}$$

$$\psi_k^-(x) = \frac{\Theta(k-k_b)}{\sqrt{2\pi}} \sqrt{\frac{k}{k'}} \begin{cases} e^{-ik'x} + a_-(k)e^{ik'x} & x \geq 0 \\ b_-(k)e^{-ikx} & x < 0 \end{cases}, \tag{17.2b}$$

where

$$a(k) = \frac{k-k'}{k+k'}; \quad a_-(k) = -\frac{k-k'}{k+k'}, \tag{17.3}$$

$$b(k) = \frac{2k}{k+k'}; \quad b_-(k) = \frac{2k'}{k+k'}, \tag{17.4}$$

$$k' = \sqrt{\frac{2m\left(E_k - V_0\right)}{\hbar^2}} = \sqrt{k^2 - k_b^2}, \tag{17.5}$$

and

$$k_b = \sqrt{\frac{2mV_0}{\hbar^2}}. \tag{17.6}$$

There are two independent eigenfunctions for a given value of

$$k = \sqrt{\frac{2mE_k}{\hbar^2}}. \tag{17.7}$$

The $\psi_k^+(x)$ eigenfunction corresponds to a wave incident from the left and the $\psi_k^-(x)$ eigenfunction to one incident from the right.

If $E_k < V_0$, then the eigenfunctions are non-degenerate and given by

$$\psi_k^+(x) = \frac{\Theta(k)}{\sqrt{2\pi}} \begin{cases} e^{ikx} + c(k)e^{-ikx} & x < 0 \\ d(k)e^{-\kappa x} & x \geq 0 \end{cases}, \tag{17.8}$$

where

$$\kappa = \sqrt{k_b^2 - k^2} \tag{17.9}$$

and

$$c(k) = \frac{k - i\kappa}{k + i\kappa} = e^{-2i\alpha(k)}; \quad \alpha(k) = \tan^{-1}\frac{\kappa}{k}, \tag{17.10}$$

$$d(k) = \frac{2k}{k + i\kappa} = \frac{2k}{\sqrt{k^2 + \kappa^2}} e^{-i\alpha(k)}. \tag{17.11}$$

17.1 Steady-State Approach

I assume that there is a single energy eigenfunction, corresponding to a wave incident from the left. The trick is to break up the probability current density associated with $\psi_k^+(x)$ into three parts, the e^{ikx} part for $x < 0$ corresponding to the incident wave, the e^{-ikx} part for $x < 0$ corresponding to the reflected wave, and the e^{ikx} or $e^{-\kappa x}$ part for $x > 0$ corresponding to the transmitted wave. Thus, the incident probability current density is calculated using $\psi_i(x) = e^{ikx}/\sqrt{2\pi}$ as

$$J_i = \frac{\hbar}{2mi}\left[\psi_i^*(x)\frac{d\psi_i(x)}{dx} - \psi_i(x)\frac{d\psi_i^*(x)}{dx}\right]$$
$$\approx \frac{\hbar}{2mi}\left[e^{-ikx}ike^{ikx} - e^{ikx}\left(-ike^{-ikx}\right)\right]\rho = \rho v_k, \tag{17.12}$$

where $\rho = 1/(2\pi)$ is the probability density associated with the incident wave and

$$v_k = \frac{\hbar k}{m}. \tag{17.13}$$

For $E > V_0$, the reflected probability current density is calculated using $\psi_r(x) = a(k)e^{-ikx}/\sqrt{2\pi}$ as

$$J_r = -\left|a(k)\right|^2 \rho v_k, \tag{17.14}$$

and the transmitted probability current density is calculated using $\psi_t(x) = b(k)e^{ik'x}/\sqrt{2\pi}$ as

$$J_t = \left|b(k)\right|^2 \rho v_k', \tag{17.15}$$

where

$$v'_k = \frac{\hbar k'}{m} = \frac{\hbar}{m}\sqrt{k^2 - k_b^2}. \tag{17.16}$$

The reflection coefficient is

$$\mathcal{R} = \frac{-J_r}{J_i} = |a(k)|^2 = \left(\frac{k-k'}{k+k'}\right)^2 \tag{17.17}$$

and the transmission coefficient is

$$\mathcal{T} = \frac{J_t}{J_i} = \frac{v'_k}{v_k}|b(k)|^2 = \frac{k'}{k}|b(k)|^2 = \frac{4kk'}{(k+k')^2}, \tag{17.18}$$

with

$$\mathcal{R} + \mathcal{T} = 1. \tag{17.19}$$

For $E_k < V_0$, the reflected probability current density is calculated using $\psi_r(x) = c(k)e^{ikx}/\sqrt{2\pi}$ as

$$J_r = -|c(k)|^2 \rho v_k = \rho v_k. \tag{17.20}$$

The reflection coefficient is

$$\mathcal{R} = \frac{-J_r}{J_i} = 1. \tag{17.21}$$

The probability current density in the barrier vanishes since the wave function is real for $x > 0$. All these results were derived previously in Chap. 6.

17.2 Time-Dependent Approach

In the time-dependent approach, the initial state wave function is expanded in terms of the stationary state eigenfunctions $\psi_k^{+,-}(x)$ to obtain the expansion coefficients $\Phi(k)$, which are then used to calculate $\psi(x,t)$ as

$$\psi(x,t) = \int_0^\infty dk \left[\Phi_+(k)\psi_k^+(x) + \Phi_-(k)\psi_k^-(x)\right] e^{-i\hbar k^2 t/2m}. \tag{17.22}$$

The integral is restricted to positive values of k since the eigenfunctions $\psi_k^{+,-}(x)$ given in Eqs. (17.2) and (17.8) are so restricted. The key point in solving the scattering problem in this fashion is to choose a wave packet incident from the left that is sufficiently broad to insure that it does not spread much on the time scale of the scattering. Moreover, it should be much broader than the distance over which the potential varies significantly (in this case the variation occurs as a step, so the packet is *always* larger in extent than the interval over which the potential changes). In other words, you want the central energy E_0 associated with the incident wave packet to be fairly well-defined. The same type of formalism can then be used for both $E_0 > V_0$ and $E_0 < V_0$.

Since the incident wave packet is localized to the left of the step and moving to the right, $\Phi_-(k) \approx 0$. Moreover, to calculate the expansion coefficients from the initial wave packet, I can neglect any of the e^{-ikx} components of the eigenfunctions $\psi_k^+(x)$ given in Eqs. (17.2a) and (17.8), respectively, since they correspond to a wave packet moving to the left. To a good approximation, the initial wave function, centered at $x = -x_0 < 0$ at time $t = 0$ can be expanded as

$$\psi(x,0) \approx \int_0^\infty dk\, \Phi_+(k)\psi_k^+(x) \approx \frac{1}{\sqrt{2\pi}}\int_{-\infty}^\infty dk\, \Phi(k)e^{ikx}, \tag{17.23}$$

where $\Phi(k)$ is a real function, sharply peaked about $k = k_0$, corresponding to energy

$$E_0 = \hbar^2 k_0^2/2m, \tag{17.24}$$

and the integral is extended to $-\infty$ based on the assumption that $\Phi(k) \approx 0$ for $k < 0$. In other words, the initial wave packet doesn't yet know about the step potential it is going to encounter, so it can be expanded in terms of *free-particle plane wave eigenfunctions*. This is a key step in solving the problem.

After a time $t \gg x_0/v_0$, with v_0 defined by

$$v_0 = \hbar k_0/m, \tag{17.25}$$

the scattering is finished. I now look at the wave function for times $t \gg x_0/v_0$.

There is one final point to note before starting the calculation. For a wave packet moving to the right with a fairly well-defined energy, I can write Eq. (17.23) as

$$\psi(x,0) \approx \frac{1}{\sqrt{2\pi}}\int_{-\infty}^\infty dk\, \Phi(k)e^{ikx} = \frac{1}{\sqrt{2\pi}}e^{ik_0x}\int_{-\infty}^\infty dk\, \Phi(k)e^{i(k-k_0)x}. \tag{17.26}$$

If $\Phi(k)$ is *symmetric* about $k = k_0$, as I shall assume, then

$$\psi(x,0) \approx \frac{1}{\sqrt{2\pi}}e^{ik_0x}\int_{-\infty}^\infty dk\, \Phi(k)\cos[(k-k_0)\,x]. \tag{17.27}$$

Without loss of generality, I can assume that the integral is positive, implying that

$$\psi(x,0) = |\psi(x,0)|\, e^{ik_0x}. \tag{17.28}$$

The phase factor gives rise to the motion of the wave packet to the right with speed $v_0 = \hbar k_0/m$.

17.2.1 $E_0 > V_0$ for Step Potential

I expand the wave function at time t in terms of the *exact* eigenfunctions, but neglect any contributions from $\psi_k^-(x)$. For $E_0 > V_0$

$$\psi(x,t) \approx \frac{1}{\sqrt{2\pi}} \int_0^\infty dk\, \Phi(k)\psi_k^+(x) e^{-ihk^2 t/2m}$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty dk\, \Phi(k) e^{-ihk^2 t/2m} \begin{cases} e^{ikx} + a(k)e^{-ikx} & x < 0 \\ b(k)e^{ik'x} & x \geq 0 \end{cases}, \tag{17.29}$$

where $\Phi(k)$ is a sharply peaked, real function centered at $k = k_0$. The calculation proceeds exactly as in Chap. 3. That is, *neglecting spreading* [i.e., approximating $k^2 = [k_0 + (k - k_0)]^2 \approx k_0^2 + 2k_0(k - k_0) = 2kk_0 - k_0^2$], I find

$$\psi(x,t) = \int_{-\infty}^\infty dk\, \Phi(k)\psi_k(x) e^{-ihk^2 t/2m} \approx \frac{1}{\sqrt{2\pi}} e^{i\hbar k_0^2 t/2m}$$
$$\times \int_{-\infty}^\infty dk\, \Phi(k) e^{-ikv_0 t} \begin{cases} e^{ikx} + a(k_0)e^{-ikx} & x < 0 \\ b(k_0)e^{ik'x} & x \geq 0 \end{cases}, \tag{17.30}$$

where $a(k)$ and $b(k)$ are evaluated at $k = k_0$. The only extra feature I have to deal with is the $e^{ik'x}$ term.

Since k' appears in an exponent and is a function of k, as is evident from Eq. (17.5), I cannot simply evaluate it at $k = k_0$, but must include a correction term as well, to insure that each term in the exponent has a magnitude much less than unity. Consequently, I expand k' around $k = k_0$ in the exponent,

$$e^{ik'x} \approx \exp\left[i \left(k_0' + \left.\frac{dk'}{dk}\right|_{k=k_0} (k - k_0) \right) x \right], \tag{17.31}$$

where

$$k_0' = \sqrt{k_0^2 - k_b^2}.$$

I then use the relationship

$$\frac{dk'}{dk} = \frac{k}{k'} \tag{17.32}$$

to evaluate

$$k_0' + \left.\frac{dk'}{dk}\right|_{k=k_0}(k-k_0) = k_0' + \frac{k_0 k}{k_0'} - \frac{k_0^2}{k_0'}, \tag{17.33}$$

and substitute this result into Eqs. (17.31) and (17.30) to arrive at

$$\psi(x,t) \approx \frac{1}{\sqrt{2\pi}} e^{i\hbar k_0^2 t/2m} \int_{-\infty}^{\infty} dk\, \Phi(k) e^{-ikv_0 t} \times \begin{cases} e^{ikx} + a(k_0)e^{-ikx} & x<0 \\ e^{i\left(k_0' - k_0^2/k_0'\right)x} b(k_0) e^{ikk_0 x/k_0'} & x \geq 0 \end{cases}. \tag{17.34}$$

Comparing Eq. (17.34) with Eq. (17.23), I find that

$$\psi(x,t) = e^{i\hbar k_0^2 t/2m} \begin{cases} \psi(x - v_0 t, 0) + a(k_0)\psi(-x - v_0 t, 0) & x<0 \\ b(k_0) e^{i\left(k_0' - k_0^2/k_0'\right)x} \psi\left[\left(\frac{k_0}{k_0'}\right)x - v_0 t, 0\right] & x \geq 0 \end{cases}. \tag{17.35}$$

Equation (17.35) gives the time-dependent wave function, neglecting spreading. I should note that the expansion of k' around $k = k_0$ breaks down when $E_k \approx V_0$. In that case, dispersion leads to a wave packet that no longer propagates without distortion. A necessary condition to neglect this dispersion is $k_0'\sigma \gg 1$, where σ is the width of the incident packet. This condition may not be sufficient, however, for certain types of wave packets and values of x.

I look at each term in Eq. (17.35) separately and remember that the original wave packet is centered at $x = -x_0 < 0$ at $t = 0$. I consider only those times $t \gg x_0/v_0$, for which the scattering is complete. The first term in the first line of Eq. (17.35), $\psi(x - v_0 t, 0)$, is peaked at

$$\begin{aligned} x_c - v_0 t &= -x_0; \\ x_c &= v_0 t - x_0, \end{aligned} \tag{17.36}$$

which corresponds to positive $x_c \gg 0$ for $t \gg x_0/v_0$. In other words,

$$\psi(x - v_0 t, 0) \approx 0 \quad \text{for } x < 0 \text{ and } t \gg x_0/v_0, \tag{17.37}$$

implying that the first term in the first line of Eq. (17.35) is approximately equal to zero for times $t \gg x_0/v_0$. The second term in the first line of Eq. (17.35), $a(k_0)\psi(-x - v_0 t, 0)$, is peaked at

$$\begin{aligned} -x_c - v_0 t &= -x_0; \\ x_c &= x_0 - v_0 t \end{aligned} \tag{17.38}$$

and corresponds to the reflected wave for $t \gg x_0/v_0$. The term in the second line of Eq. (17.35), $b(k_0)\psi\left[\left(\frac{k_0}{k_0'}\right)x - v_0 t, 0\right]$, is peaked at

$$\left(\frac{k_0}{k_0'}\right)x_c - v_0 t = -x_0;$$
$$x_c = v_0'\left(t - \frac{x_0}{v_0}\right), \tag{17.39}$$

where

$$v_0' = \frac{\hbar k_0'}{m} \tag{17.40}$$

is the speed of the transmitted wave. For $t \gg x_0/v_0$, this corresponds to the transmitted wave packet, moving with speed v_0'. Note that it takes a time

$$t_0 = x_0/v_0 \tag{17.41}$$

for the center of the initial wave packet to reach the origin.

I now return to the final result, Eq. (17.35), which gives an approximation to $\psi(x,t)$ for *all* times. I can use Eq. (17.28) to transform this equation into

$$\psi(x,t) \approx e^{-i\hbar k_0^2 t/2m}\begin{cases} e^{ik_0x}\left|\psi\left(x - v_0 t, 0\right)\right| & \\ +a(k_0)e^{-ik_0x}\left|\psi\left(-x - v_0 t, 0\right)\right| & x < 0 \\ b(k_0)e^{ik_0'x}\left|\psi\left[\left(\frac{k_0}{k_0'}\right)x - v_0 t, 0\right]\right| & x \geq 0 \end{cases}. \tag{17.42}$$

To illustrate the physical content of Eq. (17.42), I choose an initial wave packet of the form

$$\psi\left(x, 0\right) = \frac{1}{\left(\pi\sigma^2\right)^{1/4}} e^{-(x+x_0)^2/2\sigma^2} e^{ik_0x} \tag{17.43}$$

and substitute it into Eq. (17.42) to arrive at

$$\psi(x,t) \approx \frac{e^{-i\hbar k_0^2 t/2m}}{\left(\pi\sigma^2\right)^{1/4}}\begin{cases} e^{ik_0x}e^{-(x+x_0-v_0t)^2/2\sigma^2} & \\ +\,a(k_0)e^{-ik_0x}e^{-(-x+x_0-v_0t)^2/2\sigma^2} & x < 0 \\ b(k_0)e^{ik_0'x}e^{-\left[x-v_0'(t-x_0/v_0)\right]^2/2\sigma'^2} & x \geq 0 \end{cases}, \tag{17.44}$$

where

$$\sigma' = \sigma k_0'/k_0 < \sigma. \tag{17.45}$$

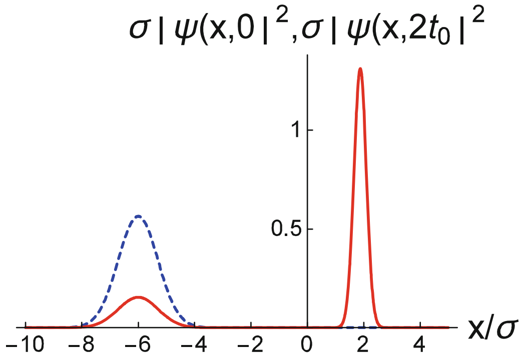

Fig. 17.3 Graphs of $\sigma\left|\psi(x,0)\right|^2$ (blue, dashed curve), along with $\left|\psi(x,t=2t_0)\right|^2$ (red, solid curve) for $k_0\sigma = 200$, $k_b\sigma = 190$, $k_0'\sigma = 62.5$, $v_0t_0/\sigma = 6$

In Fig. 17.3 I plot $\sigma\left|\psi(x,0)\right|^2$, along with $\sigma\left|\psi(x,t=2t_0)\right|^2$. The reflected and transmitted packets are seen clearly in the figure. For the dimensionless parameters $k_0\sigma = 200$, $k_b\sigma = 190$, $k_0'\sigma = 62.5$, $v_0t_0/\sigma = 6$, the peak value of $\left|\psi(x,t)\right|^2$ of the reflected wave is reduced by a factor of $\left|a(k_0)\right|^2 = 0.274$ and that of the transmitted wave is increased by a factor of $\left|b(k_0)\right|^2 = 2.32$. Moreover, since $\sigma' < \sigma$, the transmitted packet is compressed, as was the classical particle density shown in Fig. 17.3, and the speed of the transmitted wave packet is reduced by a factor of $k_0'/k_0 = 0.31$. Although the amplitude of the transmitted packet is larger than that of the incident packet, the transmitted probability current density is less than that of the initial packet, as I now show.

I can use Eqs. (17.42) and (5.139) to show that the probability current density associated with the incident wave packet is approximately

$$\begin{aligned} J_i &= \frac{\hbar}{2mi}\left[\psi_i^*(x,t)\frac{d\psi_i(x,t)}{dx} - \psi_i(x,t)\frac{d\psi_i^*(x,t)}{dx}\right] \\ &= \frac{\hbar}{2mi}\left[\left|\psi^*(x-v_0t,0)\right|e^{-ik_0x}\frac{d\left(\left|\psi(x-v_0t,0)\right|e^{ik_0x}\right)}{dx}\right] + \text{c.c.} \\ &\approx \frac{\hbar}{2mi}\left[ik_0\left|\psi(x-v_0t,0)\right|^2\right] + \text{c.c.} = v_0\left|\psi(x-v_0t,0)\right|^2, \end{aligned} \tag{17.46}$$

where $\psi_i(x,t)$ corresponds to the incident wave packet *before* it reaches the barrier. In deriving Eq. (17.46), I assumed that $k_0\sigma \gg 1$, consistent with the assumption that the incident wave packet is sharply peaked in momentum space. Similarly,the reflected probability current density for times well after the packet has scattered from the barrier is approximately

$$J_r = -\left|a(k_0)\right|^2 v_0\left|\psi\left[x+v_0t,0\right]\right|^2. \tag{17.47}$$

and the transmitted probability current density is

$$J_t = |b(k_0)|^2 \, v_0' \left| \psi \left[\left(\frac{k_0}{k_0'} \right) x - v_0 t, 0 \right] \right|^2 . \tag{17.48}$$

Since $|b(k_0)|^2 \, v_0' < v_0$, the maximum transmitted current density is less than the maximum incident current density.

The reflection coefficient is equal to the magnitude of time-integrated reflected probability current density (this is what a detector placed in the path of the particle would measure) divided by the time-integrated initial probability current density

$$\mathcal{R} = \frac{-\int J_r dt}{\int J_i dt} = \frac{|a(k_0)|^2 \, v_0}{v_0} = |a(k_0)|^2 = \left(\frac{k_0 - k_0'}{k_0 + k_0'} \right)^2 \tag{17.49}$$

and the transmission coefficient is

$$\mathcal{T} = \frac{\int J_t dt}{\int J_i dt} = \frac{|a(k_0)|^2 \, v_0'}{v_0} = \frac{k_0'}{k_0} |b(k_0)|^2 = \frac{4 k_0 k_0'}{\left(k_0 + k_0' \right)^2} < 1. \tag{17.50}$$

These results agree with the steady-state approach.

17.2.2 $E_0 < V_0$ *for Step Potential*

For $E_0 < V_0$

$$\begin{aligned} \psi(x,t) &\approx \int_0^\infty dk \, \Phi(k) \psi_k^+(x) e^{-i\hbar k^2 t/2m} \\ &\approx \int_{-\infty}^\infty dk \, \Phi(k) e^{-i\hbar k^2 t/2m} \begin{cases} e^{ikx} + c(k) e^{-ikx} & x < 0 \\ d(k) e^{-\kappa x} & x \geq 0 \end{cases} . \end{aligned} \tag{17.51}$$

The calculation proceeds as before, except that there are a few wrinkles. You might think that all that is necessary is to replace k' by $i\kappa$ and k_0' by $i\kappa_0$ but you would be wrong on two counts. First, for $x > 0$, the major contribution to the integral over k may no longer be centered at $k = k_0$, even though $\Phi(k)$ is peaked at $k = k_0$. The reason for this is that the eigenfunction for $x > 0$ is an exponentially decreasing function of $\kappa x = \sqrt{k_b^2 - k^2} x$, so it is possible to get a relatively larger contribution to the integral over k near $k = k_b$ rather than $k = k_0$. In general, the integral in Eq. (17.51) must be done numerically for $x > 0$. On the other hand, for the scattering problem I am interested in calculating the wave function only when $t \gg t_0 = x_0/v_0$, times for which the wave function in the region $x > 0$ is negligibly small. Thus I neglect the region $x > 0$ in my analysis of the problem, at least for the moment.

The second problem with replacing k' by $i\kappa$ and k_0' by $i\kappa_0$ is linked to the fact that, while $a(k)$ and $b(k)$ are real, $c(k)$ and $d(k)$ are complex; that is,

$$c(k) = e^{-i\phi(k)}; \tag{17.52a}$$

$$d(k) = \frac{2k}{\sqrt{k^2+\kappa^2}} e^{-i\phi(k)/2}; \tag{17.52b}$$

$$\phi(k) = 2\alpha(k) = 2\tan^{-1}(\kappa/k) = 2\tan^{-1}\left(\sqrt{k_b^2-k^2}/k\right). \tag{17.52c}$$

When a function appears in an exponent and you expand the function, only terms that are much less than unity can be neglected. I cannot simply replace $\phi(k)$ by $\phi(k_0)$. Instead, I must expand it as

$$\phi(k) \approx \phi(k_0) + \frac{d\phi}{dk_0}(k-k_0) \tag{17.53}$$

where

$$\frac{d\phi}{dk_0} = \left.\frac{d\phi}{dk}\right|_{k=k_0} = -\frac{2}{\kappa_0} \tag{17.54}$$

and

$$\kappa_0 = \sqrt{\frac{2m(V_0-E_0)}{\hbar^2}}. \tag{17.55}$$

Using this result and Eq. (17.621) in Eq. (17.51) with $k^2 \approx -k_0^2 + 2k_0 k$, I find for $x<0$,

$$\begin{aligned}
\psi(x,t) &\approx e^{i\hbar k_0^2 t/2} m\psi(x-v_0t,0) + e^{i\hbar k_0^2 t/2} e^{-i\phi(k_0)+ik_0\frac{d\phi}{dk_0}} \\
&\quad\times \int_{-\infty}^{\infty} dk\, \Phi(k) e^{-ikv_0t} e^{-ikx} e^{-ik\frac{d\phi}{dk_0}} \\
&= e^{i\hbar k_0^2 t/2}\psi(x-v_0t,0) \\
&\quad + e^{i\hbar k_0^2 t/2} e^{-i\phi(k_0)+ik_0\frac{d\phi}{dk_0}} \psi\left(-x-v_0t-\frac{d\phi}{dk_0},0\right) \\
&= e^{-i\hbar k_0^2 t/2} e^{ik_0x} \left|\psi(x-v_0t,0)\right| \\
&\quad + e^{-i\hbar k_0^2 t/2} e^{-i\phi(k_0)} e^{-ik_0x} \left|\psi\left(-x-v_0t-\frac{d\phi}{dk_0},0\right)\right|.
\end{aligned} \tag{17.56}$$

Since

$$\frac{d\phi}{dk_0} = \frac{d\phi}{dE_0}\frac{dE_0}{dk_0} = \frac{\hbar^2 k_0}{m}\frac{d\phi}{dE_0} = \hbar v_0 \frac{d\phi}{dE_0} = -\frac{2}{\kappa_0}, \tag{17.57}$$

it follows that the reflected wave packet is centered at

$$-x_c - v_0\left(t + \hbar\frac{d\phi}{dE}\right) = -x_0;$$
$$x_c = x_0 - v_0\left(t + \hbar\frac{d\phi}{dE}\right), \tag{17.58}$$

or

$$x_c = x_0 - v_0\left(t - \frac{2}{\kappa_0 v_0}\right). \tag{17.59}$$

There is a *time delay* in the scattering given by

$$t_d = -\frac{1}{v_0}\frac{d\phi}{dk_0} = -\hbar\frac{d\phi}{dE_0} = \frac{2}{\kappa_0 v_0} = \frac{\hbar}{\sqrt{E\left(V_0 - E\right)}}. \tag{17.60}$$

The delay is proportional to $\hbar$—this is a quantum effect. How can we interpret this time delay? In the stationary state approach to the scattering problem, the probability current density vanishes for $x > 0$. In the wave packet approach, however, it cannot vanish at all times. There must be a positive probability current density up until the time the center of the wave packet reaches the step and a negative probability current density as the (time delayed) wave packet is reflected. It is as if the packet is checking out the potential barrier and then decides it does not have enough energy to be transmitted so it goes back from whence it came, but it takes a time delay for the wave packet to figure this out. The probability current density at the origin, given by

$$J(x=0,t) = \frac{i\hbar}{2m}\left[\psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x} - \psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\right]_{x=0}, \tag{17.61}$$

with $\psi(x,t)$ given by Eq. (17.56) and $\psi(x,0)$ by Eq. (17.43), is plotted in Fig. 17.4 in units of $v_0/\left(\sqrt{\pi}\right)$ as a function of $v_0 t/\sigma$ for $x_0/\sigma = 6$, $k_b\sigma = 200$ and $k_0\sigma = 190, 100$. You can see that the curve has a "dispersion-like" form, even though it is not exactly proportional to the derivative of the wave packet envelope. The peak amplitude of the curve and the time delay decrease with increasing k_b/k_0. In the low energy limit $k_b/k_0 \sim \infty$, $J(0,t) \sim 0$ and $t_d \sim 0$. The time delay is largest when $E \approx V_0$; in this limit, the wave function penetrates significantly into the barrier.

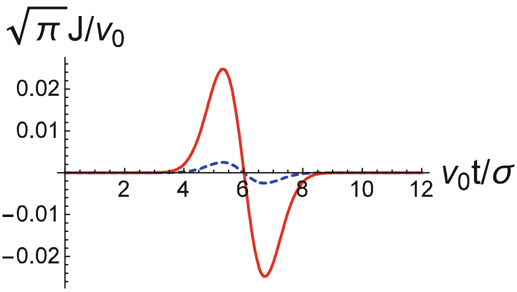

Fig. 17.4 Probability current density at $x = 0$ in dimensionless units as a function of $v_0 t/\sigma$ for $x_0/\sigma = 6$ and $k_b\sigma = 200$. The red solid curve is for $k_0\sigma = 190$ and the blue dashed curve for $k_0\sigma = 100$

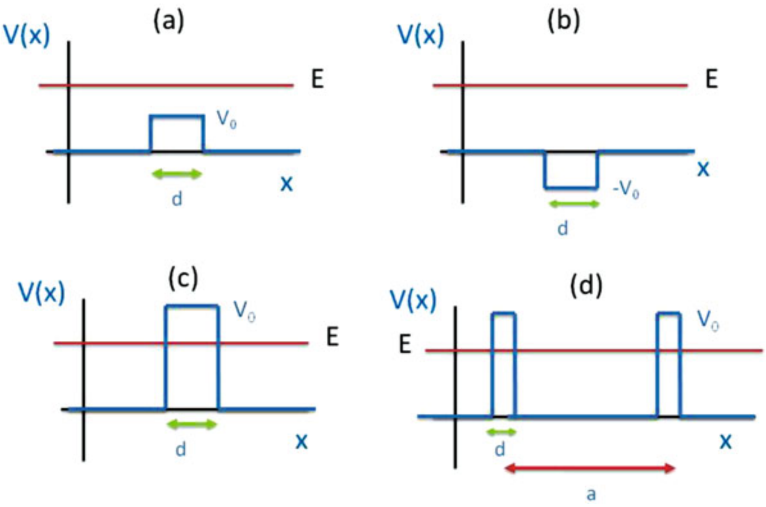

Fig. 17.5 Different piecewise constant potentials and incident scattering energies

Similar analyses can be used for different potentials. I will describe in qualitative terms what happens in each of the cases shown in Fig. 17.5.

Cases (a) and (b) are analogous to an optical field incident normally on a thin dielectric film. There is constructive interference in reflection when twice the film thickness, $2d$, is a half integral number of wavelengths and destructive interference when it is an integral number of wavelengths. The transmission goes to unity at positions of destructive interference in reflection. The resonances can be very narrow if the index of refraction is high. In the quantum-mechanical problem, you can also have very narrow transmission resonances as a function of $k_0'd$. In the scattering problem, such resonances are accompanied by large time delays. To avoid wave packet spreading and to see these resonances, you must take the width of the initial wave packet to be much larger than the barrier width, *multiplied* by the number of "bounces" the packet makes in the region of the potential. The number of "bounces" is simply the barrier width d divided by $v_0' t_d$.

In case (c), there can be quantum-mechanical tunneling through the barrier. There is also a time delay in this problem, but no resonance phenomena. The wave function simply builds up and decays inside the barrier.

Case (d) is perhaps the most interesting. It corresponds to a Fabry-Perot filter for light. If each barrier has a very small transmission coefficient separately, *the transmission coefficient for the double barrier can approach unity when the incoming wavelength corresponds to a standing wave pattern between the two barriers*! This is the result found from the steady-state approach. How can this be? How can the wave penetrate significantly through the first barrier since it doesn't even *know* about the second barrier? The answer to this question is "It can't" if the width of the packet is much less than a, the separation of the barriers. In that case, the wave packet is partially transmitted by the barrier, but mostly reflected by it. The part that is transmitted bounces back and forth between the barriers, leaking out a little bit each time. Thus, the transmitted wave is a *series* of packets, as is the reflected wave, with the time between reflected or transmitted packets equal to the round-trip time in the cavity.

How then does a Fabry-Perot filter work? In order to see the narrow resonances, you must choose an initial wave packet that is much larger than the distance a between the barriers, multiplied by number of bounces in the cavity, $a/(v_0 t_d)$, which can be enormous. The time delay near resonance is inversely proportional to the transmission coefficient for a *single* barrier. In other words, you need an incoming packet that is quasi-monochromatic to see the narrow resonances. Part of the packet penetrates through the barrier, is reflected from the second barrier, and interferes with subsequent transmission through the barrier. After a long time, a steady state standing wave pattern is formed in the cavity having an intensity that is much larger than that of the incident wave—the part that leaks out the other end has an intensity equal to the initial wave intensity. After *very* long times, the initial wave packet can be almost totally transmitted by the double barrier.

17.3 Summary

We have seen several interesting features of scattering from one-dimensional potentials. Both steady-state and time-dependent approaches were used. In some sense, the time-dependent approach provides a justification for the equations for the reflection and transmission coefficients used in the steady-state approach and provides a prescription for obtaining the time delay from the phase of the steady-state eigenfunctions. I now turn my attention to scattering from spherically symmetric potentials.

17.4 Problems

1. How does one-dimensional scattering by a step potential differ for classical and quantum-mechanical scattering of a particle? What is the optical analogue of scattering by an attractive square well? Why would you expect resonances in this case?

2. In the time-dependent scattering approach I assumed that a wave packet with a fairly well-defined energy was incident on the potential step from the left. If the energy is greater than the step height, there could be contributions to the wave function from the eigenfunctions given in Eq. (17.2b). Prove that such contributions are negligible at all times. Moreover, prove that the contribution for the e^{-ikx} part of the $\psi_k^+(x)$ eigenfunction makes a negligible contribution to $\Phi_+(k)$.

3–5. (a) Consider classical scattering of a particle having mass m by a square well potential for which $V(x) = -V_0 < 0$ for $|x| \leq a/2$ and is zero otherwise. A particle is incident from the left with energy $E = mv_0^2/2$. Show that, compared to the case when there is no potential, there is a negative time delay (that is the particle reaches a point $x > 0$ faster than it would in the absence of the potential) given by

$$t_d^{cl} = -\frac{a}{v_0} + \frac{a}{v_0'},$$

where $v_0' = \sqrt{2m(E + V_0)}$

(b) Now consider the analogous quantum problem for the scattering of a quasi-monoenergetic wave packet having energy centered at $E_0 = mv_0^2/2 = \hbar^2 k_0^2/2m$. The (amplitude) reflection and transmission coefficients for a mono-energetic wave packet having energy $E = \hbar k$ are given in Eqs. (6.107) with k_E replaced by k. If you write these coefficients as

$$R(k) = |R(k)|\, e^{i\phi_R(k)}; \qquad T(k) = |T(k)|\, e^{i\phi_T(k)},$$

show that the quantum time delays for the reflected and transmitted packets are given by

$$t_d^R = -\frac{1}{v_0}\frac{d\phi_R}{dk_0};$$

$$t_d^T = \frac{1}{v_0}\frac{d\phi_T}{dk_0}.$$

(c) Plot the intensity transmission coefficient as a function of $y = k_0 a$ for $\beta = \sqrt{2mV_0/\hbar^2}a = 500$ and $0 < y < 120$. Show that there are narrow resonances when

$$k_0'a = \sqrt{\frac{2m\left(E_0 + V_0\right)}{\hbar^2}}a = n\pi$$

for integer $n > \beta/\pi$.

(d) Plot the classical time delay and the quantum transmission time delay on the same graph in units of $a/v_0 = ma^2/\hbar y$ as a function of $y = k_0 a$ for $\beta = 500$ and $0 < y < 120$. Show that, at the position of the resonances, the quantum delay is *greater* than the classical delay. This supports the contention that the particle "bounces" back and forth in as it is scattered near resonance.

(e) In the low energy limit, $y \ll 1$, show that the time delay is given by

$$t_d^T = -\frac{ma^2}{\hbar y}\left(1 + \frac{2\cot\beta}{\beta}\right).$$

It follows from Eqs. (6.88) and (6.89) that, for $y \ll 1$, a new bound state appears near zero energy whenever $\beta = n\pi$. Thus the time delay diverges near such resonances. Since the phase varies rapidly in such regions, there is considerable dispersion and the picture of a transmitted, time-delayed, undistorted wave packet is no longer valid.[1]

6. Calculate the time delay in transmission of the scattering of a quasi-monoenergetic wave packet of a particle having mass m by a delta function potential barrier,

$$V(x) = V_0 a\delta\left(x\right)$$

where V_0, d, and a are positive constants. Show that it vanishes in the limit $\hbar \to 0$.

7–8. Consider scattering of a particle having mass m by a one-dimensional potential

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

where V_0, d, and a are positive constants.

(a) Calculate and plot the intensity transmission coefficient $\mathcal{T} = |T|^2$ as a function of $y = kd$ ($k = \sqrt{2mE/\hbar^2}$) for $\beta'^2 = 2mV_0 ad/\hbar^2 = 100$ in the strong barrier limit,

$$\frac{\beta^2}{2ka} = \frac{mV_0 a^2}{ka\hbar^2} = \frac{\beta'^2}{2y} \gg 1.$$

[1]The dependence of the time delay on β is similar to that encountered in the dependence of the scattering length (the scattering length is discussed in Chap. 18) on magnetic field strength when the field is used to tune the energy in an open scattering channel to that of a bound state in a closed channel of the intermolecular potentials. Such *Feshbach resonances* play an important role in controlling interactions in Bose-Einstein condensates [for a review, see the article by C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, *Feshbach resonances in ultracold gases,* Reviews of Modern Physics **82**, 1225–1286 (2010)].

Show that there are resonances where the transmission goes to unity and interpret your result.

(b) From the expression for the transmission amplitude T calculate and plot the scattering time delay, in units of $d/v = md^2/\hbar y$, experienced by a quasi-monoenergetic wave packet as a function of y. Show that, at the position of the resonances, the time delay goes through a maximum. Interpret your results. The time delay in these units is the number of bounces the particle makes before being scattered.

9. Consider the scattering of a quasi-monoenergetic wave packet having central energy $E = \hbar^2 k^2/2m$ by the potential

$$V(x) = \begin{cases} V_0 a\delta(x) & x < d \\ \infty & x > d \end{cases},$$

where V_0 and a are positive constants and m is the particle's mass. Plot the time delay in units of $d/v = md^2/\hbar y$ as a function of $y = ka$ for $\beta'^2 = 2mV_0 ad/\hbar^2 = 100$ in the strong barrier limit, $\beta'^2/2y \gg 1$, and interpret your results. The time delay in these units is the number of bounces the particle makes before being scattered.