

## Chapter 4

The door beckoned, so he pushed through it. Even the street was better lit. He didn't know how, he just knew—the patron seated at the corner table was his man. Spectacles, unkept hair, old sweater, one bottle, one glass. Elbows on the bar and foot on the rail, he strained for calmness until the barkeep finally appeared. A meek “bourbon, rocks,” left his lips, then he shuffled a bill he thought was a five onto the bar, pocketed the change, tugged on the drink, and let his feet move him to the corner table. “I wanna talk to you....” The stranger slowly greeted him with his eyes, as if he was expected, and replied “What about, son?” Resisting the urge to look away, the words just fell “. . .those Rutherford rays. . .”

# Scattering in One Dimension

The free state addressed in the last chapter is the simplest problem because the potential is chosen to be zero. The next simplest problems are those where the potentials are piecewise constant. A potential that is piecewise constant is discontinuous at one or more points. The potential is chosen to be zero in one region and is of non-zero value in other regions without a transition region. A discontinuity in a potential is not completely realistic though these problems do model some realistic systems well. Transistors, semiconductors, and alpha decay (Rutherford rays) are examples for which an abrupt change in potential is a key feature. Though they are not perfect models, piecewise constant potentials do contain some realistic physics and serve to illustrate features of potentials that are very steep.

The primary reason to address these problems is that a discontinuous change in potential is much more mathematically tractable than a continuous change. These problems are usually addressed using the position space, time-independent form of the Schrodinger equation. The strategy is to divide space into regions at the locations where the potential changes and then attain a solution for each region. The points at which the potential changes are boundaries. The wavefunction and its first derivative must be the same on both sides of the boundaries. Equating the wavefunctions and their first derivatives at the boundaries provides a system of equations that yield descriptive information. Also, solving problems in one dimension is usually mathematically attractive and can be realistic. One dimensional situations are often a precursor to multi-dimensional situations.

There is some key quantum mechanical behavior in these problems. You should absorb the idea that a particle has a non-zero probability to appear on the other side of a potential barrier that it does not classically have the energy to surmount. This is known as **barrier penetration** or **tunneling**. Also, a particle has a non-zero probability to be reflected at any boundary regardless of energy. For instance, a particle possessing enough energy to surmount a potential barrier can still be reflected. You should learn the terms **reflection and transmission coefficients**.

A particle is in either a **free state** (chapter 3), a **bound state** (chapter 5, 6, and parts of others), or a **scattering state**. The bound state is described by a potential that holds a particle for a non-zero time period. The scattering state can be described as an interaction of a free particle with a potential that results in a free particle. If a free particle interacts with the potential and does not become bound, the particle is in a scattering state. The hydrogen atom may be ionized. The electron can escape and enter a free state, but it cannot escape without the influence of an external photon. Scattering concerns the situation where there is no external influence.

Finally, you should also appreciate the presence of the postulates of quantum mechanics.

Though the position space, time-independent Schrodinger equation dominates the discussion, remember that it is simply a convenient form of the sixth postulate.

1. Find the reflection and transmission coefficients for a particle of energy  $E > V_0$  incident from the left on the vertical step potential

$$V(x) = \begin{cases} 0 & \text{if } x < 0 \quad \text{region 1,} \\ V_0 & \text{if } x > 0 \quad \text{region 2.} \end{cases}$$

Notice that region 2 extends to infinity. This is an approximation to a potential that is very steep but not perfectly vertical, and of significant though not of infinite width. If the step is not vertical, it is difficult to match boundary conditions, and if the step is not of infinite extent, “tunneling” (see problem 3) is possible.

Particles that are incident from the left will either be reflected or transmitted. The **reflection coefficient**, denoted  $R$ , is classically defined as the ratio of intensity reflected to intensity incident. The classical **transmission coefficient**, denoted  $T$ , is the ratio of intensity transmitted to intensity incident. Quantum mechanically, intensity is analogous to probability density. Quantum mechanical transmission and reflection coefficients are based on probability density flux (problem 2). The reflection and transmission coefficients must sum to 1 in either classical or quantum mechanical regimes.

The two physical boundary conditions applicable to this and many other boundary value problems are *the wave function and its first derivative are continuous*.

A general solution to the Schrodinger equation for a particle approaching from the left is

$$\psi_1(x) = A e^{ik_1x} + B e^{-ik_1x}, \quad x < 0,$$

$$\psi_2(x) = C e^{ik_2x}, \quad x > 0,$$

where the subscripts on the wavefunctions and wave numbers indicate regions 1 or 2, and

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \quad \text{and} \quad k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}.$$

The  $k_i$  are real because  $E > V_0$ . In region 1, the term  $A e^{ik_1x}$  is the incident wave and  $B e^{-ik_1x}$  describes the reflected wave.  $C e^{ik_2x}$  models the transmitted wave in region 2. A term like  $D e^{-ik_2x}$ , modeling a particle moving to the left in region 2, is not physically meaningful for a particle given to be incident from the left. Equivalently,  $D = 0$  for the same reason. Applying the boundary condition that the wavefunction is continuous,

$$\psi_1(0) = \psi_2(0) \Rightarrow A e^0 + B e^0 = C e^0 \Rightarrow A + B = C.$$

The derivative of the wavefunction is

$$\psi'_1(x) = A i k_1 e^{ik_1x} - B i k_1 e^{-ik_1x}, \quad x < 0,$$

$$\psi_2'(x) = C i k_2 e^{i k_2 x}, \quad x > 0,$$

so continuity of the first derivative means

$$\psi_1'(0) = \psi_2'(0) \Rightarrow A i k_1 e^{i k_1(0)} - B i k_1 e^{-i k_1(0)} = C i k_2 e^{i k_2(0)} \Rightarrow k_1(A - B) = k_2 C.$$

We now have two equations in the three unknowns  $A$ ,  $B$ , and  $C$ . Eliminating  $C$ ,

$$k_1(A - B) = k_2(A + B) \Rightarrow (k_1 - k_2)A = (k_1 + k_2)B \Rightarrow B = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)A.$$

From this relation we can calculate the reflection coefficient. The incident probability density is

$$|A e^{i k_1 x}|^2 = (A e^{i k_1 x})^* (A e^{i k_1 x}) = (A^* e^{-i k_1 x})(A e^{i k_1 x}) = A^* A e^0 = |A|^2,$$

or the intensity of the incident wave is the square of the norm of the coefficient of the incident wave. Similarly, the intensity of the reflected wave is  $|B|^2$ , and the intensity of the transmitted wave is  $|C|^2$ . In this specific problem the reflection coefficient is

$$R = \frac{|B|^2}{|A|^2} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 |A|^2 / |A|^2 = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \quad \text{and}$$

$$R + T = 1 \Rightarrow T = 1 - R = 1 - \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 = \left(\frac{k_1 + k_2}{k_1 + k_2}\right)^2 - \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 = \frac{4k_1 k_2}{(k_1 + k_2)^2}.$$

**Postscript:** Classically,  $R = 0$  and  $T = 1$  if  $E > V_0$ . Figure 4–2 illustrates the quantum

mechanical analogy. What does it mean that  $R > 0$  when  $E > V_0$ ? For a single particle, it means that a portion of the wavefunction is transmitted and a portion of the wavefunction is reflected. Postulate 4 says that you can calculate the probabilities for finding the particle in region 1 or 2 from the probability amplitudes, but can do no better. If you look, you will find the particle in either region 1 or region 2 per postulate 3, and the measurement will leave the state vector in the eigenstate corresponding to the location that you measured per postulate 5. The probability of finding the particle in the other region is then zero.

Notice that the particle will have longer wavelength and thus less momentum in region 2 since the energy relative to the “floor” of the potential is less in region 2 than region 1.

The classical trajectory of a particle is continuous and a change in trajectory (the first derivative) will be continuous. Quantum mechanically, refined arguments are necessary. The validity of the two boundary conditions can be demonstrated for a Gaussian wavefunction. The issue becomes that a wave packet that is quantized in wave number will scatter from a potential with precisely the same reflection and transmission coefficients as a Gaussian wavefunction. This can be done for a wave packet quantized in wave number that is still smooth compared to the scale of the

potential variations. This is a non-trivial calculation that is beyond our scope. The point is that the boundary conditions of continuity of the wavefunction and its first derivative are also justified quantum mechanically.

2. (a) Calculate the amplitude  $C$  of the transmitted portion of the wavefunction in terms of the coefficient  $A$  for the vertical step potential of problem 1.

(b) Show that the ratio  $|C|^2/|A|^2$  is  $\neq T$  from problem 1.

(c) Rectify the discrepancy between part (b) and the result of problem 1.

Parts (a) and (b) are intended to demonstrate a counter-intuitive fact that is explained in part (c). Use intermediate results from problem 1 to solve for  $C$  in terms of  $A$ . Form the ratio  $|C|^2/|A|^2$  which is not the same as  $T$  from problem 1. Part (c) requires that you know that flux is velocity times intensity. Since the particle has a different height above the floor of the potential in regions 1 and 2, it has not only a different wavenumber but a different velocity. These velocities are related to the de Broglie relation. The ratio  $v_2|C|^2/v_1|A|^2$  is the transmission coefficient found in problem 1.

(a) Using intermediate results from problem 1, the amplitude of the transmitted portion is

$$C = A + B = A + \left(\frac{k_1 - k_2}{k_1 + k_2}\right) A = \left(\frac{k_1 + k_2}{k_1 + k_2}\right) A + \left(\frac{k_1 - k_2}{k_1 + k_2}\right) A = \left(\frac{2k_1}{k_1 + k_2}\right) A.$$

(b) The ratio of the squares of the magnitudes is not the transmission coefficient of problem 1,

$$\frac{|C|^2}{|A|^2} = \left(\frac{2k_1}{k_1 + k_2}\right)^2 |A|^2 / |A|^2 = \frac{4k_1^2}{(k_1 + k_2)^2} \neq \frac{4k_1k_2}{(k_1 + k_2)^2}.$$

(c) These differ because the energy, and thus the velocity, of the wave changes as the particle crosses the step. Flux is intensity times velocity. Probability density flux, probability density times velocity, is appropriate for a quantum mechanical description. Since  $v_i = \frac{p_i}{m} = \frac{\hbar k_i}{m}$ ,

$$T = \frac{v_2|C|^2}{v_1|A|^2} = \frac{\hbar k_2/m|C|^2}{\hbar k_1/m|A|^2} = \frac{k_2|C|^2}{k_1|A|^2} = k_2 \left(\frac{2k_1}{k_1 + k_2}\right)^2 |A|^2 / k_1 |A|^2 = \frac{4k_1k_2}{(k_1 + k_2)^2},$$

consistent with the problem 1.

**Postscript:** A reflected wave is the same height above the floor of the potential as the incident wave so the reflected wave has the same energy, velocity, and wave number as the incident wave. The velocities cancel in region 1 so are not considered in calculating the reflection coefficient, *i.e.*,

$$R = \frac{v_1|B|^2}{v_1|A|^2} = \frac{|B|^2}{|A|^2}.$$

3. Determine the transmission coefficient for a particle with  $E < V_0$  incident from the left on the rectangular barrier

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

If the energy of the particle is less than the height of the step, and the “potential plateau” is of finite length, the particle incident from the left can appear on the right side of a barrier. This is a non-classical phenomena known as **barrier penetration** or **tunneling**. Classically, if a ball is rolled up a ramp of height  $h$  with kinetic energy  $K$ , the ball will roll back down the ramp if  $K < mgh$ . A quantum mechanical ball has a non-zero probability that the ball would appear on the other side of the ramp in the case  $K < mgh$ .

This is a boundary value problem with three regions because there are two boundaries. The strategy is to require continuity of the wavefunction and its first derivative at all boundaries and solve for the transmission coefficients in terms of the ratios of the squares of the appropriate wavefunction coefficients.

(a) Divide “all space” into three regions at the boundaries of the potential  $\pm a$ . The wavefunctions consist of a linear combination of waves in both directions in each of the three regions:

$$\begin{aligned} \psi_1(x) &= A e^{ikx} + B e^{-ikx} & \text{for } x < -a, \\ \psi_2(x) &= C e^{\kappa x} + D e^{-\kappa x} & \text{for } -a < x < a, \\ \psi_3(x) &= F e^{ikx} + G e^{-ikx} & \text{for } x > a, \end{aligned}$$

where  $k = \sqrt{2mE} / \hbar$  and  $\kappa = \sqrt{2m(V_0 - E)} / \hbar$ . Notice that  $\kappa$  is defined so that it is real for  $E < V_0$ . This is a technique that leads to minor simplifications. Conclude that  $G = 0$  because it is the coefficient of an oppositely directed incident wave, and therefore, is not physical.

(b) Apply the boundary condition that the wavefunction must be continuous at the boundaries. This yields two equations. Differentiate the wavefunction and then apply the boundary condition that the first derivative of the wavefunction must be continuous at boundaries. This yields two more equations. Eliminating  $B$  from the two equations for the left boundary, you should find

$$2A e^{-ika} = \left(1 - \frac{i\kappa}{k}\right) C e^{-\kappa a} + \left(1 + \frac{i\kappa}{k}\right) D e^{\kappa a}.$$

Using the two equations at the right boundary to solve for two of the unknown coefficients in terms of the coefficient  $F$ , you should find

$$C e^{\kappa a} = \frac{1}{2} \left(1 + \frac{ik}{\kappa}\right) F e^{ika} \quad \text{and} \quad D e^{-\kappa a} = \frac{1}{2} \left(1 - \frac{ik}{\kappa}\right) F e^{ika}.$$

(c) Use the last two equations to eliminate the coefficients  $C$  and  $D$  from the first equation so

$$A e^{-ika} = F e^{ika} \left[ \cosh(2\kappa a) + \frac{i(\kappa^2 - k^2)}{2k\kappa} \sinh(2\kappa a) \right].$$

Remember that  $\sinh(x) = \frac{e^x - e^{-x}}{2}$  and  $\cosh(x) = \frac{e^x + e^{-x}}{2}$ .

(d) A reflected and transmitted particle will be the same height above the floor of the defined potential so the transmission coefficient is the ratio of probability density of that portion of the wavefunction which “goes through” the barrier, represented by  $|F|^2$ , to the incident probability density, represented by  $|A|^2$ . The reciprocal of this ratio,  $|A|^2/|F|^2$ , is

$$T^{-1} = 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2\left(\frac{2a}{\hbar} \sqrt{2m(V_0 - E)}\right),$$

which is a more pleasing and compact expression than  $T$  that still indicates  $T \neq 0$  when  $E < V_0$ .

(a) For the region  $x > a$ ,  $\psi(x) = F e^{ikx} + G e^{-ikx}$ , and  $G = 0$  because it is the coefficient of an oppositely directed incident wave that cannot be physical. So the wave function is

$$\psi(x) = \begin{cases} A e^{ikx} + B e^{-ikx}, & \text{for } x < -a, \\ C e^{\kappa x} + D e^{-\kappa x}, & \text{for } -a < x < a, \\ F e^{ikx}, & \text{for } x > a, \end{cases}$$

where  $k = \sqrt{2mE}/\hbar$  and  $\kappa = \sqrt{2m(V_0 - E)}/\hbar$ .

(b) There are three regions so there are two boundaries. Continuity at the boundaries requires

$$A e^{-ika} + B e^{ika} = C e^{-\kappa a} + D e^{\kappa a}, \quad x = -a, \quad \text{and} \quad (1)$$

$$C e^{\kappa a} + D e^{-\kappa a} = F e^{ika}, \quad x = a, \quad (2)$$

so there are two equations in five unknowns. The derivative of  $\psi(x)$  is

$$\psi'(x) = \begin{cases} A ik e^{ikx} - B ik e^{-ikx}, & \text{for } x < -a, \\ C \kappa e^{\kappa x} - D \kappa e^{-\kappa x}, & \text{for } -a < x < a, \\ F ik e^{ikx}, & \text{for } x > a. \end{cases}$$

Applying the boundary condition of continuity of the first derivative at  $x = -a$ ,

$$A ik e^{-ika} - B ik e^{ika} = C \kappa e^{-\kappa a} - D \kappa e^{\kappa a}, \quad \text{and at } x = a, \quad (3)$$

$$C \kappa e^{\kappa a} - D \kappa e^{-\kappa a} = F ik e^{ika}. \quad (4)$$

There are now four equations in five unknowns. Multiplying equation (1) by  $ik$ ,

$$B ik e^{ika} = C ik e^{-\kappa a} + D ik e^{\kappa a} - A ik e^{-ika}.$$

Substituting this into equation (3) for  $B ik e^{ika}$ ,

$$A ik e^{-ika} - C ik e^{-\kappa a} - D ik e^{\kappa a} + A ik e^{-ika} = C \kappa e^{-\kappa a} - D \kappa e^{\kappa a}$$

$$\begin{aligned} \Rightarrow \quad 2A ik e^{-ika} &= C ik e^{-\kappa a} + C \kappa e^{-\kappa a} + D ik e^{\kappa a} - D \kappa e^{\kappa a} \\ &= C (ik + \kappa) e^{-\kappa a} + D (ik - \kappa) e^{\kappa a} \end{aligned}$$

$$\Rightarrow 2A e^{-ika} = \left(1 - \frac{i\kappa}{k}\right) C e^{-\kappa a} + \left(1 + \frac{i\kappa}{k}\right) D e^{\kappa a}. \quad (5)$$

Multiplying equation (2) by  $\kappa$  and solving for the term with the coefficient  $D$ ,

$$D \kappa e^{-\kappa a} = F \kappa e^{ika} - C \kappa e^{\kappa a}$$

Substituting the right side into equation (4) for  $D \kappa e^{-\kappa a}$ ,

$$\begin{aligned} C \kappa e^{\kappa a} - F \kappa e^{ika} + C \kappa e^{\kappa a} &= F i k e^{ika} \\ \Rightarrow 2C \kappa e^{\kappa a} &= F \kappa e^{ika} + F i k e^{ika} = F (\kappa + ik) e^{ika} \\ \Rightarrow C e^{\kappa a} &= \frac{1}{2} \left(1 + \frac{ik}{\kappa}\right) F e^{ika}. \end{aligned} \quad (6)$$

Multiplying equation (2) by  $\kappa$  and solving for the term with the coefficient  $C$ ,

$$C \kappa e^{\kappa a} = F \kappa e^{ika} - D \kappa e^{-\kappa a}$$

Substituting the right side into equation (4) for  $C \kappa e^{\kappa a}$ ,

$$\begin{aligned} F \kappa e^{ika} - D \kappa e^{-\kappa a} - D \kappa e^{-\kappa a} &= F i k e^{ika} \\ -2D \kappa e^{-\kappa a} &= -F \kappa e^{ika} + F i k e^{ika} = F (-\kappa + ik) e^{ika} \\ \Rightarrow D e^{-\kappa a} &= \frac{1}{2} \left(1 - \frac{ik}{\kappa}\right) F e^{ika}. \end{aligned} \quad (7)$$

(c) The signs on the exponentials in equations (6) and (7) are opposite those in equation (5), so

$$\begin{aligned} C e^{\kappa a} &= \frac{1}{2} \left(1 + \frac{ik}{\kappa}\right) F e^{ika} \quad \Rightarrow \quad C e^{-\kappa a} = \frac{1}{2} \left(1 + \frac{ik}{\kappa}\right) F e^{ika} e^{-2\kappa a}, \\ D e^{-\kappa a} &= \frac{1}{2} \left(1 - \frac{ik}{\kappa}\right) F e^{ika} \quad \Rightarrow \quad D e^{\kappa a} = \frac{1}{2} \left(1 - \frac{ik}{\kappa}\right) F e^{ika} e^{2\kappa a}, \end{aligned}$$

and now the signs of the exponentials are consistent. Substituting these into equation (5),

$$\begin{aligned} \Rightarrow 2A e^{-ika} &= \left(1 - \frac{i\kappa}{k}\right) \frac{1}{2} \left(1 + \frac{ik}{\kappa}\right) F e^{ika} e^{-2\kappa a} + \left(1 + \frac{i\kappa}{k}\right) \frac{1}{2} \left(1 - \frac{ik}{\kappa}\right) F e^{ika} e^{2\kappa a} \\ &= \frac{F e^{ika}}{2} \left(1 - \frac{i\kappa}{k} + \frac{ik}{\kappa} + \frac{\kappa k}{\kappa k}\right) e^{-2\kappa a} + \frac{F e^{ika}}{2} \left(1 + \frac{i\kappa}{k} - \frac{ik}{\kappa} + \frac{\kappa k}{\kappa k}\right) e^{2\kappa a} \\ &= \frac{F e^{ika}}{2} \left(2e^{-2\kappa a} - \frac{i\kappa}{k} e^{-2\kappa a} + \frac{ik}{\kappa} e^{-2\kappa a} + 2e^{2\kappa a} + \frac{i\kappa}{k} e^{2\kappa a} - \frac{ik}{\kappa} e^{2\kappa a}\right) \\ &= \frac{F e^{ika}}{2} \left[2(e^{-2\kappa a} + e^{2\kappa a}) - \frac{ik^2}{k\kappa} e^{-2\kappa a} + \frac{ik^2}{k\kappa} e^{-2\kappa a} + \frac{ik^2}{k\kappa} e^{2\kappa a} - \frac{ik^2}{k\kappa} e^{2\kappa a}\right] \\ &= \frac{F e^{ika}}{2} \left[2(e^{-2\kappa a} + e^{2\kappa a}) + \frac{ik^2}{k\kappa} (e^{2\kappa a} - e^{-2\kappa a}) - \frac{ik^2}{k\kappa} (e^{2\kappa a} - e^{-2\kappa a})\right] \\ &= F e^{ika} \left[2 \left(\frac{e^{2\kappa a} + e^{-2\kappa a}}{2}\right) + \frac{i(\kappa^2 - k^2)}{k\kappa} \left(\frac{e^{2\kappa a} - e^{-2\kappa a}}{2}\right)\right] \end{aligned}$$

$$\Rightarrow A e^{-ika} = F e^{ika} \left[ \cosh(2\kappa a) + \frac{i(\kappa^2 - k^2)}{2k\kappa} \sinh(2\kappa a) \right].$$

(d) The transmission coefficient is the ratio of intensity transmitted, represented by  $|F|^2$ , to the intensity incident, represented by  $|A|^2$ . It is conventional to calculate the reciprocal of this ratio to arrive at a compact expression. Both sides are in the polar form of complex numbers, *i.e.*, magnitude and phase. The last result can be arranged as the ratio

$$\left| \frac{A e^{-ika}}{F e^{ika}} \right| = \left| \left[ \cosh(2\kappa a) + \frac{i(\kappa^2 - k^2)}{2k\kappa} \sinh(2\kappa a) \right] \right|.$$

$$\text{Now } \left| \frac{A e^{-ika}}{F e^{ika}} \right| = \left[ \frac{A e^{-ika}}{F e^{ika}} \frac{A^* e^{ika}}{F^* e^{-ika}} \right]^{1/2} = \left[ \frac{A A^*}{F F^*} \right]^{1/2} = \frac{[A A^*]^{1/2}}{[F F^*]^{1/2}} = \frac{|A|}{|F|}$$

$$\Rightarrow \frac{|A|^2}{|F|^2} = \left| \left[ \cosh(2\kappa a) + \frac{i(\kappa^2 - k^2)}{2k\kappa} \sinh(2\kappa a) \right] \right|^2 = \cosh^2(2\kappa a) + \left( \frac{(\kappa^2 - k^2)}{2k\kappa} \right)^2 \sinh^2(2\kappa a),$$

where we have used the fact the product of complex conjugates is sum of the squares of the real part and the coefficient of the imaginary part. Recalling that  $\cosh^2(x) = 1 + \sinh^2(x)$ ,

$$\begin{aligned} \frac{|A|^2}{|F|^2} &= 1 + \sinh^2(2\kappa a) + \left( \frac{\kappa^4 - 2k^2\kappa^2 + k^4}{4k^2\kappa^2} \right) \sinh^2(2\kappa a) \\ &= 1 + \left( 1 + \frac{\kappa^4 - 2k^2\kappa^2 + k^4}{4k^2\kappa^2} \right) \sinh^2(2\kappa a) \\ &= 1 + \left( \frac{4k^2\kappa^2 + \kappa^4 - 2k^2\kappa^2 + k^4}{4k^2\kappa^2} \right) \sinh^2(2\kappa a) \\ &= 1 + \left( \frac{\kappa^4 + 2k^2\kappa^2 + k^4}{4k^2\kappa^2} \right) \sinh^2(2\kappa a) \\ &= 1 + \frac{(\kappa^2 + k^2)^2}{4k^2\kappa^2} \sinh^2(2\kappa a). \end{aligned}$$

Substituting  $k = \sqrt{2mE}/\hbar$  and  $\kappa = \sqrt{2m(V_0 - E)}/\hbar$ ,

$$\begin{aligned} \frac{|A|^2}{|F|^2} &= 1 + \frac{\left( \frac{2m}{\hbar^2}(V_0 - E) + \frac{2m}{\hbar^2}E \right)^2}{4 \left( \frac{2m}{\hbar^2}E \right) \left( \frac{2m}{\hbar^2}(V_0 - E) \right)} \sinh^2 \left( \frac{2a}{\hbar} \sqrt{2m(V_0 - E)} \right) \\ &= 1 + \frac{\frac{4m^2}{\hbar^4} (V_0 - E + E)^2}{\frac{4m^2}{\hbar^4} 4E(V_0 - E)} \sinh^2 \left( \frac{2a}{\hbar} \sqrt{2m(V_0 - E)} \right) \\ \Rightarrow \frac{|A|^2}{|F|^2} &= T^{-1} = 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2 \left( \frac{2a}{\hbar} \sqrt{2m(V_0 - E)} \right). \end{aligned}$$

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4. Determine the transmission coefficient for a particle with  $E = V_0$  incident from the left on the rectangular barrier defined in the last problem.

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The intent of this problem is to further develop your skills applying boundary conditions. Require continuity of the wavefunction and its first derivative at all boundaries.

The first step, which is non-trivial, is to write a proper wavefunction. Similar to problem 3, the wavefunction in the three regions can be written as

$$\begin{aligned}\psi_1(x) &= A e^{ikx} + B e^{-ikx} & \text{for } x < -a, \\ \psi_2(x) &= C + D x & \text{for } -a < x < a, \\ \psi_3(x) &= F e^{ikx} & \text{for } x > a.\end{aligned}$$

The wave number is the same in regions 1 and 3 because particle energy is the same height above the “floor,” and is zero in region 2 for either possible definition because  $E = V_0$ . Follow parts (b) through (d) of problem 3 to get the reciprocal of the transmission coefficient,

$$T^{-1} = 1 + \frac{2mE}{\hbar^2} a^2.$$

When  $E = V_0$ , the wavenumber in the region  $-a < x < a$  is  $k = \sqrt{2m(V_0 - E)}/\hbar = 0$ , so

the wavefunction can be written 
$$\psi(x) = \begin{cases} A e^{ikx} + B e^{-ikx}, & \text{for } x < -a, \\ C + D x, & \text{for } -a < x < a, \\ F e^{ikx}, & \text{for } x > a. \end{cases}$$

Continuity of the wavefunction at  $x = -a$  means

$$A e^{-ika} + B e^{ika} = C - D a, \tag{1}$$

$$\text{and at } x = a, \quad C + D a = F e^{ika}. \tag{2}$$

Continuity of the derivative of the wavefunction at  $x = -a$  means

$$A i k e^{-ika} - B i k e^{ika} = D, \tag{3}$$

$$\text{and at } x = a, \quad D = F i k e^{ika}. \tag{4}$$

Multiplying equation (1) by  $ik$  and solving for the term with the coefficient  $B$  yields

$$B i k e^{ika} = ik C - ik D a - A i k e^{-ika}.$$

Substituting this into equation (3) eliminates the unknown coefficient  $B$ ,

$$\begin{aligned}A i k e^{-ika} - ik C + ik D a + A i k e^{-ika} &= D \\ \Rightarrow 2A i k e^{-ika} &= ik C + D(1 - ika).\end{aligned} \tag{5}$$

Equation (2) can be written  $C = F e^{ika} - D a$ , and substituting this into equation (5),

$$\begin{aligned}2A i k e^{-ika} &= ik(F e^{ika} - D a) + D(1 - ika) \\ &= ik F e^{ika} - ik D a + D(1 - ika) \\ &= ik F e^{ika} + D(1 - 2ika).\end{aligned}$$

Substituting equation (4) into the last equation eliminates the unknown coefficient  $D$ ,

$$\begin{aligned}
 2A ik e^{-ika} &= ik F e^{ika} + F ik e^{ika} (1 - 2ika) \\
 \Rightarrow 2A e^{-ika} &= F e^{ika} + F e^{ika} (1 - 2ika) \\
 \Rightarrow 2A e^{-ika} &= F e^{ika} (2 - 2ika) \\
 \Rightarrow A e^{-ika} &= F e^{ika} (1 - ika) \\
 \Rightarrow \frac{A e^{-ika}}{F e^{ika}} &= 1 - ika \\
 \text{and } \left| \frac{A e^{-ika}}{F e^{ika}} \right| &= \left| \frac{A}{F} \right| = \frac{|A|}{|F|} \quad \text{as previously shown,} \\
 \Rightarrow \frac{|A|^2}{|F|^2} &= |1 - ika|^2 = 1 + k^2 a^2.
 \end{aligned}$$

Substituting  $k = \sqrt{2mE}/\hbar$ ,  $\frac{|A|^2}{|F|^2} = T^{-1} = 1 + \frac{2mE}{\hbar^2} a^2$  for  $E = V_0$ .

5. Show in the limit  $E \rightarrow V_0$  from below, that the results of problems 3 and 4 are equivalent.

The intent of this problem is to demonstrate self-consistency by examining a limiting case. It is a technique that is difficult to teach and important to learn. Start with the result of problem 3. Expand  $\sinh(x)$  and ignore the higher order terms so that  $\sinh(x) \approx x$  since  $E \approx V_0$ . Of course, in the limit  $E \rightarrow V_0$  the results of problem 3 and 4 must be the same.

Start with the reciprocal of the transmission coefficient from problem 3. Ignoring higher order terms as negligible in the series expansion of  $\sinh(x) \Rightarrow \sinh(x) \approx x$ ,

$$\begin{aligned}
 T^{-1} &= 1 + \frac{V_0^2}{4E(V_0 - E)} \left( \frac{2a}{\hbar} \sqrt{2m(V_0 - E)} \right)^2 \\
 &= 1 + \frac{V_0^2}{4E(V_0 - E)} \left( \frac{4a^2}{\hbar^2} 2m(V_0 - E) \right) \\
 &= 1 + \frac{V_0^2}{E} \left( \frac{a^2}{\hbar^2} 2m \right) \\
 &= 1 + \frac{2mV_0^2}{\hbar^2 E} a^2.
 \end{aligned}$$

Remembering that  $E \approx V_0$ ,  $T^{-1} \approx 1 + \frac{2mE}{\hbar^2} a^2$ .

6. (a) A particle of energy  $E > V_0$  is incident on a rectangular barrier of width  $2a$ . Solve for the value of the transmission coefficient and locate the positions of the maxima and minima in terms of wave number. Plot transmission coefficient versus barrier width for a particle of constant energy and variable barrier width.

- (b) Locate the positions of the maxima in terms of particle energy. Plot transmission coefficient versus particle energy where  $E > V_0$  and barrier width is fixed.

This problem introduces a phenomenon known as **resonance scattering**. At certain values of particle wave number (energy), there is 100% transmission and no reflection. Part (a) should illustrate resonance scattering for an incident particle of fixed energy and a barrier width that is varied. Part (b) illustrates the same phenomenon where particle energy is varied and barrier width is fixed. Start with an intermediate result from problem 10,

$$\frac{1}{T} = 1 + \frac{1}{4} \left( \frac{k_1^2 - k_2^2}{k_1 k_2} \right)^2 \sin^2(2k_2 a).$$

Solve for  $T$  instead of its reciprocal. The maxima occur where the sine term is zero at barrier widths of  $2a = n\pi/k_2$ . The minima occur where the sine term is one, where the transmission coefficient has the value  $T = \left( \frac{2k_1 k_2}{k_1^2 + k_2^2} \right)^2$ . Part (b) is likely easiest if started with

$$\frac{1}{T} = 1 + \frac{V_0^2}{4E(E - V_0)} \sin^2 \left( \frac{2a}{\hbar} \sqrt{2m(E - V_0)} \right),$$

the result of problem 10 in terms of energy. Again, solve for  $T$  instead of its reciprocal. This plot is more difficult because the independent variable  $E$  appears in five places including the square root of the sine squared term. The important part of this graph is the shape. If you do not have access to a commercial graphing package, try to imagine what the graph should look like, and skip to the solution. You should find the maxima at

$$E = \frac{\pi^2 \hbar^2}{8ma^2} n^2 + V_0.$$

This result is closely related to the infinite square well that is encountered in the next chapter.

$$\begin{aligned} \text{(a)} \quad \frac{1}{T} &= 1 + \frac{1}{4} \left( \frac{k_1^2 - k_2^2}{k_1 k_2} \right)^2 \sin^2(2k_2 a) = \frac{4k_1^2 k_2^2}{4k_1^2 k_2^2} + \frac{k_1^4 - 2k_1^2 k_2^2 + k_2^4}{4k_1^2 k_2^2} \sin^2(2k_2 a) \\ &= \frac{4k_1^2 k_2^2 + (k_1^4 - 2k_1^2 k_2^2 + k_2^4) \sin^2(2k_2 a)}{4k_1^2 k_2^2} \\ \Rightarrow T &= \frac{4k_1^2 k_2^2}{4k_1^2 k_2^2 + (k_1^4 - 2k_1^2 k_2^2 + k_2^4) \sin^2(2k_2 a)}. \end{aligned}$$

Maxima of  $T = 1$  occur where  $\sin^2(2k_2 a) = 0$ , *i.e.*, where  $2k_2 a = n\pi \Rightarrow 2a = \frac{n\pi}{k_2}$  are the barrier widths at which maxima occur, noting that the width of the barrier is given to be  $2a$ . The minima occur where the sine squared term is one, so minima occur at

$$T = \frac{4k_1^2 k_2^2}{4k_1^2 k_2^2 + (k_1^4 - 2k_1^2 k_2^2 + k_2^4) \cdot 1} = \frac{4k_1^2 k_2^2}{k_1^4 + 2k_1^2 k_2^2 + k_2^4} \Rightarrow T = \left( \frac{2k_1 k_2}{k_1^2 + k_2^2} \right)^2 \text{ at minima.}$$

(b) In terms of particle energy,

$$\begin{aligned} \frac{1}{T} &= 1 + \frac{V_0^2}{4E(E - V_0)} \sin^2 \left( \frac{2a}{\hbar} \sqrt{2m(E - V_0)} \right) \\ &= \frac{4E(E - V_0) + V_0^2 \sin^2 \left( \frac{2a}{\hbar} \sqrt{2m(E - V_0)} \right)}{4E(E - V_0)} \\ \Rightarrow T &= \frac{4E(E - V_0)}{4E(E - V_0) + V_0^2 \sin^2 \left( \frac{2a}{\hbar} \sqrt{2m(E - V_0)} \right)}. \end{aligned}$$

The maxima occur where the sine squared term is zero, so

$$\begin{aligned} \frac{2a}{\hbar} \sqrt{2m(E - V_0)} &= n\pi \Rightarrow \sqrt{2m(E - V_0)} = \frac{n\pi\hbar}{2a} \\ \Rightarrow 2m(E - V_0) &= \frac{\pi^2\hbar^2}{4a^2} n^2 \Rightarrow E - V_0 = \frac{\pi^2\hbar^2}{8ma^2} n^2 \\ \Rightarrow E &= \frac{\pi^2\hbar^2}{8ma^2} n^2 + V_0 \end{aligned}$$

which are energies that are closely related to the eigenenergies of a particle in an infinite square well.

**Postscript:** Resonance scattering is the circumstance where 100% transmission occurs.

7. (a) Show in position space that

$$\Delta(\psi'(x)) = \frac{2m}{\hbar^2} \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} V(x) \psi(x) dx$$

is the general value of the discontinuity in the first derivative for an infinite potential.

(b) Calculate the value of the discontinuity in the first derivative for a particle interacting with the potential well  $V(x) = -\alpha \delta(x)$ .

Use the conditions that  $\psi$  and  $\psi'$  are continuous at any boundary of a finite potential. There must, however, be a discontinuity in the first derivative at all infinite boundaries. If the value of the discontinuity can be calculated, the boundary condition for the first derivative is again useful. The method of calculating the value of the discontinuity is to put the potential into the Schrodinger equation, integrate around the infinite boundary, and let the limits approach zero from both sides.

For a general potential  $V(x)$ , the Schrodinger equation in position space is

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x).$$

If we integrate around the point which is the discontinuity, this is

$$-\frac{\hbar^2}{2m} \int_{-\epsilon}^{\epsilon} \frac{d^2 \psi(x)}{dx^2} dx + \int_{-\epsilon}^{\epsilon} V(x) \psi(x) dx = E \int_{-\epsilon}^{\epsilon} \psi(x) dx,$$

which assumes that the infinite boundary is at  $x = 0$ . The quantity  $\epsilon$  is infinitesimal. If we let  $\epsilon \rightarrow 0$ , the right side of the equation is zero. The integral of a finite quantity,  $\psi(x)$ , over an arbitrarily small interval is zero. The term with the potential does not vanish because the integral of an infinite quantity, the potential, can be non-zero even for an arbitrarily small interval. So,

$$\begin{aligned} \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} \frac{d^2 \psi(x)}{dx^2} dx &= \frac{2m}{\hbar^2} \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} V(x) \psi(x) dx \\ \Rightarrow \left. \frac{d\psi(x)}{dx} \right|_{\epsilon \rightarrow 0} - \left. \frac{d\psi(x)}{dx} \right|_{-\epsilon \rightarrow 0} &= \frac{2m}{\hbar^2} \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} V(x) \psi(x) dx \\ \Rightarrow \Delta(\psi'(x)) &= \frac{2m}{\hbar^2} \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} V(x) \psi(x) dx \end{aligned} \quad (1)$$

is the general value of the discontinuity in the first derivative.

(b) A delta function potential is infinite, so employing equation (1),

$$\Delta(\psi'(x)) \Big|_{x=0} = \frac{2m}{\hbar^2} \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} (-\alpha \delta(x)) \psi(x) dx = -\frac{2m}{\hbar^2} \alpha \psi(0),$$

because regardless of how closely  $\epsilon$  approaches zero,  $-\epsilon < 0 < \epsilon$  meaning that zero remains within the limits of integration. Since the value of the delta function that makes its argument zero is within the limits of integration, the integral is the wavefunction evaluated at the point that makes the argument of the delta function zero.

**Postscript:** An infinite potential models a perfectly rigid and perfectly impenetrable wall. The wavefunction must be zero at an infinite potential barrier and in the region of infinite potential because the term  $V\psi$  in the Schrodinger equation would be infinite otherwise. There is a non-smooth “corner” in the wavefunction as it goes to zero at any position other than  $\pm\infty$ , thus there is a discontinuity in the first derivative of the wavefunction. This physically unrealistic model is useful to understanding concepts, is mathematically tractable, and is a first approximation to an abrupt and large potential.

8. Calculate the reflection and transmission coefficients for a particle incident on the potential

$$V(x) = -\alpha \delta(x).$$

This problem is intended to demonstrate how a potential that includes a delta function is treated specifically, and how to treat a discontinuity in general. First, write the wavefunction for two regions because the delta function is of “zero” width. The wavenumber is the same in regions 1 and 2 because the particle energy is the same height above the potential “floor” in both regions. A  $\psi(0)$  is required. Use either  $\psi_1(0)$  or  $\psi_2(0)$ , because the condition of continuity of the wavefunction at the boundary ensures that they are the same. We use  $\psi_2(0)$  because it has one fewer terms than  $\psi_1(0)$ . Classically, the reflection coefficient must be zero. The quantum mechanical result is non-zero.

The solution to the Schrodinger equation in position space is

$$\psi_1(x) = A e^{ikx} + B e^{-ikx}, \quad x < 0, \quad \psi_2(x) = C e^{ikx}, \quad x > 0,$$

where the infinite potential well is at  $x = 0$ . Continuity of the wave function means

$$A e^{ik(0)} + B e^{-ik(0)} = C e^{ik(0)} \Rightarrow A + B = C.$$

The first derivatives in regions 1 and 2 are

$$\psi'_1(x) = ik A e^{ikx} - ik B e^{-ikx}, \quad \psi'_2(x) = ik C e^{ikx}.$$

We calculated the general value of the discontinuity of the first derivative in problem 7. This is the difference of the first derivatives in regions 1 and 2, meaning

$$\begin{aligned} \psi'_1(0) - \psi'_2(0) &= -\frac{2m}{\hbar^2} \alpha \psi(0) \\ \Rightarrow ik A e^{ik(0)} - ik B e^{-ik(0)} - ik C e^{ik(0)} &= -\frac{2m}{\hbar^2} \alpha \psi(0). \end{aligned}$$

Using  $\psi_2(0) = C$ ,

$$\begin{aligned} ik A - ik B - ik C &= -\frac{2m}{\hbar^2} \alpha C \\ \Rightarrow ik A - ik B &= C \left( ik - \frac{2m}{\hbar^2} \alpha \right), \end{aligned}$$

and we use the continuity condition,  $A + B = C$ , to eliminate  $C$ , so

$$\begin{aligned} ik A - ik B &= (A + B) \left( ik - \frac{2m}{\hbar^2} \alpha \right) \\ \Rightarrow ik A - ik B &= A \left( ik - \frac{2m}{\hbar^2} \alpha \right) + B \left( ik - \frac{2m}{\hbar^2} \alpha \right) \\ \Rightarrow A \left( ik - ik + \frac{2m}{\hbar^2} \alpha \right) &= B \left( ik + ik - \frac{2m}{\hbar^2} \alpha \right) \\ \Rightarrow A \left( \frac{2m}{\hbar^2} \alpha \right) &= B \left( 2ik - \frac{2m}{\hbar^2} \alpha \right) \\ \Rightarrow B &= A \left[ \left( \frac{2m}{\hbar^2} \alpha \right) / \left( 2ik - \frac{2m}{\hbar^2} \alpha \right) \right] = \frac{m\alpha A}{ik\hbar^2 - m\alpha}. \end{aligned}$$

The reflection coefficient is

$$R = \frac{|B|^2}{|A|^2} = \left( \frac{m\alpha A^*}{-ik\hbar^2 - m\alpha} \right) \left( \frac{m\alpha A}{ik\hbar^2 - m\alpha} \right) \frac{1}{|A|^2} = \frac{m^2\alpha^2}{k^2\hbar^4 + m^2\alpha^2} = \frac{1}{1 + k^2\hbar^4/m^2\alpha^2}.$$

The transmission coefficient is

$$T = 1 - R = 1 - \frac{m^2\alpha^2}{k^2\hbar^4 + m^2\alpha^2} = \frac{k^2\hbar^4 + m^2\alpha^2 - m^2\alpha^2}{k^2\hbar^4 + m^2\alpha^2} = \frac{k^2\hbar^4}{k^2\hbar^4 + m^2\alpha^2} = \frac{1}{1 + m^2\alpha^2/k^2\hbar^4}.$$

**Postscript:** Any curve that has a sharp corner has a discontinuity in its next order derivative. Delta functions and theta functions can be useful in describing discontinuities. Techniques seen in problems 7 and 8 are useful in a number of areas, the use of delta functions in particular is becoming increasingly popular, and you will see these techniques in future chapters.

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## Practice Problems

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9. For a particle that encounters a vertical step potential of height  $V_0$ , calculate the reflection and transmission coefficients for the particle energies (a)  $E = 2V_0$ , (b)  $E = 3V_0/2$ , (c)  $E = 1.1V_0$ , and (d)  $E = V_0$ . (e) Explain the result of part (d).

---

This problem is intended primarily to reinforce the quantum mechanical effect that reflection occurs at a step even when  $E > V_0$ . It should further familiarize you with reflection and transmission coefficients. The boundary value problem for a vertical step potential is solved in problem 1, resulting in the general forms of the reflection and transmission coefficients

$$R = \left( \frac{k_1 - k_2}{k_1 + k_2} \right)^2 \quad \text{and} \quad T = 1 - R = \frac{4k_1 k_2}{(k_1 + k_2)^2}.$$

Express the energies of parts (a) through (d) in terms of the wavenumbers to attain the reflection and transmission coefficients using these equations. You should find an increasing amount of reflection as the energy of the particle gets closer to the energy of the potential barrier, until at  $E = V_0$ , the transmission coefficient is zero. The reason for this is there are artificialities built into the model to make it more mathematically tractable. Reread the comments on tunneling to identify the particular artificiality which founds the 100% reflection of part (d) to answer part (e).

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10. Determine the transmission coefficient for a particle with  $E > V_0$  incident from the left on the rectangular barrier defined in problem 3.

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Reflection from a potential barrier of energy less than that of the incident particle is another solely quantum mechanical phenomenon. Start with the wavefunction

$$\psi(x) = \begin{cases} A e^{ik_1 x} + B e^{-ik_1 x}, & \text{for } x < -a, \\ C e^{ik_2 x} + D e^{-ik_2 x}, & \text{for } -a < x < a, \\ F e^{ik_1 x}, & \text{for } x > a. \end{cases}$$

Require continuity of the wavefunction and its first derivative at all boundaries. Follow the procedures of problem 2. Define  $k_1 = \sqrt{2mE}/\hbar$  and  $k_2 = \sqrt{2m(E - V_0)}/\hbar$ , to find

$$T^{-1} = 1 + \frac{V_0^2}{4E(E - V_0)} \sin^2 \left( \frac{2a}{\hbar} \sqrt{2m(E - V_0)} \right).$$

---

11. Show in the limit  $E \rightarrow V_0$  from above, that the result of problems 4 and 10 are equivalent.

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This problem has the same intent as problem 5. Start with the result of problem 10. Expand  $\sin(x)$  and ignore the higher order terms so that  $\sin(x) \approx x$  since  $E \approx V_0$ . You must find that in the limit  $E \rightarrow V_0$  the results of problems 10 and 4 are the same.

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12. A particle of  $E > 0$  approaches the negative vertical step potential

$$V(x) = \begin{cases} 0, & \text{for } x < 0, \\ -V_0 & \text{for } x > 0. \end{cases}$$

What are the reflection and transmission coefficients if  $E = V_0/3$ , and  $E = V_0/8$ ?

---

This problem parallels the discussion of the vertical step potential. It is intended to reinforce the methods of addressing a boundary value problem. It also illustrates another completely non-classical phenomenon. Classically, we expect the reflection coefficients to be zero for any  $E > 0$ .

(a) Write the wavefunction. You have only two regions to consider. You should recognize that the general form of the wavefunction is

$$\begin{aligned} \psi_1(x) &= Ae^{ik_1x} + Be^{-ik_1x} & \text{for } x < 0, \\ \psi_2(x) &= Ce^{ik_2x} + De^{-ik_2x} & \text{for } x > 0, \end{aligned}$$

where  $k_1 = \sqrt{2mE}/\hbar$  and  $k_2 = \sqrt{2m(E - (-V_0))}/\hbar = \sqrt{2m(E + V_0)}/\hbar$ . Can you conclude that  $D = 0$  because it is the coefficient of an oppositely directed incident wave?

(b) Apply the continuity conditions to the wavefunction and its first derivative at  $x = 0$ . You should have two equations in three unknowns. The square of the coefficient  $A$  is the intensity of incidence, and the square of the coefficient  $B$  is the intensity of reflection. Since  $A$  and  $B$  are the two coefficients you want to compare, you should combine your two equations to eliminate  $C$ . You should find that

$$A(k_1 - k_2) = B(k_1 + k_2).$$

(c) The reflection coefficient is the ratio  $|B|^2/|A|^2$ , which you can form from your result of part (b). Use the definitions of the wavenumbers to establish  $R$  in terms of  $E$  and  $V_0$ , then substitute  $E = V_0/3$  and  $E = V_0/8$  to get numerical answers. You should find  $R = 1/9$  and  $1/4$ , respectively, and the transmission coefficients follow directly using  $R + T = 1$ .

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13. (a) Find the transmission coefficient for the rectangular well

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

(b) Show that  $T = 1$  in the limit that  $V_0 = 0$ .

---



This problem is provided to give you some practice at solving a boundary value problem. The procedures for this problem strongly parallel problems 3 and 4. You should find

$$T^{-1} = 1 + \frac{V_0^2}{4E(E + V_0)} \sin^2 \left( \frac{2a}{\hbar} \sqrt{2m(E + V_0)} \right)$$

using  $k_1 = \sqrt{2mE}/\hbar$  and  $k_2 = \sqrt{2m(E - (-V_0))}/\hbar = \sqrt{2m(E + V_0)}/\hbar$ . Consider the width of the well when  $V_0 \rightarrow 0$  for part (b).

14. The transmission coefficient a particle of  $E < V_0$  approaching a rectangular barrier is

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2 \left( \frac{2a}{\hbar} \sqrt{2m(V_0 - E)} \right)}.$$

- (a) Show that the term  $\frac{V_0^2}{4E(V_0 - E)} \sinh^2 \left( \frac{2a}{\hbar} \sqrt{2m(V_0 - E)} \right)$  is non-negative and real, and  
 (b) show that this means  $R < 1$  for the case  $E < V_0$ .

The transmission coefficient is non-zero for the case  $E < V_0$ , which is nonsense in a classical regime. Since quantum mechanics “lives” in the world of complex numbers, this problem shows that a non-zero transmission coefficient at a barrier is not a “trick” associated with complex or imaginary numbers, and thus, there is actually a portion transmitted and only a portion reflected when  $E < V_0$ . Start with the result of problem 3. There are energies, intrinsically positive and real, two squares, and a product to consider. Can any of those make this term negative? Once you know that the given term is non-negative and real, set it equal to a constant. Part (b) is the algebra of showing that if the constant is positive and real,  $R$  is necessarily less than one.

15. Plot barrier width versus transmission coefficient for a rectangular barrier of width  $2a$  for the case  $E = V_0$ . What widths of the barrier result in 10%, 1%, 0.1%, and 0.01% transmission when particle energy is equal to barrier height?

This problem illustrates that even a thin barrier prevents most transmission at  $E = V_0$ . A barrier a few wavelengths in width results in miniscule transmission. Start with the reciprocal of the transmission coefficient from problem 4 expressed in terms of energy and half barrier width. Use the de Broglie relationship to express the energy in terms of wavelength, then solve for  $2a$ . The barrier width that results in 10% transmission is slightly less than one particle wavelength.

16. Calculate the reflection and transmission coefficients for a particle incident on the potential

$$V(x) = \alpha \delta(x).$$

Problems 16 and 17 are intended to reinforced the ideas and the procedures in problems 7 and 8. You should find the same reflection and transmission coefficients as found in problem 8.

17. Calculate the reflection and transmission coefficients for a particle incident on the potential

$$V(x) = -\alpha \delta(x - a).$$

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Again, follow problems 7 and 8. Again, you should find the same reflection and transmission coefficients as found in problem 8 though the delta function located at other than zero requires carrying exponentials. For instance,

$$B = \frac{m\alpha A e^{i2ka}}{ik\hbar^2 - m\alpha}.$$

Remember that a norm is the square root of the product of complex conjugates per problem 3 (d).

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## Chapter 4 Homework Solutions

10. For the case  $E > V_0$ , the development is very similar to that of  $E < V_0$ . The primary differences are all exponentials have imaginary factors, and we “add zero,” add and subtract the same quantity, to arrive at a form of the transmission coefficient analogous to the case of  $E < V_0$ . The wave function is

$$\psi(x) = \begin{cases} A e^{ik_1 x} + B e^{-ik_1 x}, & \text{for } x < -a, \\ C e^{ik_2 x} + D e^{-ik_2 x}, & \text{for } -a < x < a, \\ F e^{ik_1 x}, & \text{for } x > a, \end{cases}$$

where  $k_1 = \sqrt{2mE}/\hbar$  and  $k_2 = \sqrt{2m(E - V_0)}/\hbar$ . Note since  $E > V_0$ , we define the wave number in terms of  $E - V_0$  in the region  $-a < x < a$  versus  $V_0 - E$  in the case  $E < V_0$ . The derivative is

$$\psi'(x) = \begin{cases} A i k_1 e^{ik_1 x} - B i k_1 e^{-ik_1 x}, & \text{for } x < -a, \\ C i k_2 e^{ik_2 x} - D i k_2 e^{-ik_2 x}, & \text{for } -a < x < a, \\ F i k_1 e^{ik_1 x}, & \text{for } x > a. \end{cases}$$

The continuity conditions are at  $x = -a$ ,

$$A e^{-ik_1 a} + B e^{ik_1 a} = C e^{-ik_2 a} + D e^{ik_2 a}, \quad (1)$$

and at  $x = a$ ,

$$C e^{ik_2 a} + D e^{-ik_2 a} = F e^{ik_1 a}. \quad (2)$$

Applying the boundary condition of continuity of the derivative at  $x = -a$ ,

$$A i k_1 e^{-ik_1 a} - B i k_1 e^{ik_1 a} = C i k_2 e^{-ik_2 a} - D i k_2 e^{ik_2 a}. \quad (3)$$

At  $x = a$ ,

$$C i k_2 e^{ik_2 a} - D i k_2 e^{-ik_2 a} = F i k_1 e^{ik_1 a}. \quad (4)$$

Multiplying equation (1) by  $ik_1$  and solving for the term with the coefficient of  $B$ ,

$$B i k_1 e^{ik_1 a} = C i k_1 e^{-ik_2 a} + D i k_1 e^{ik_2 a} - A i k_1 e^{-ik_1 a}.$$

Substituting the right side into equation (3),

$$\begin{aligned} A i k_1 e^{-ik_1 a} - C i k_1 e^{-ik_2 a} - D i k_1 e^{ik_2 a} + A i k_1 e^{-ik_1 a} &= C i k_2 e^{-ik_2 a} - D i k_2 e^{ik_2 a} \\ \Rightarrow 2A k_1 e^{-ik_1 a} &= C (k_1 + k_2) e^{-ik_2 a} + D (k_1 - k_2) e^{ik_2 a} \\ \Rightarrow 2A e^{-ik_1 a} &= C \left( \frac{k_1 + k_2}{k_1} \right) e^{-ik_2 a} + D \left( \frac{k_1 - k_2}{k_1} \right) e^{ik_2 a}. \end{aligned} \quad (5)$$

Multiplying equation (2) by  $ik_2$  and solving for the term with the coefficient of  $D$ ,

$$D i k_2 e^{-ik_2 a} = F i k_2 e^{ik_1 a} - C i k_2 e^{ik_2 a}.$$

Substituting this into equation (4),

$$C i k_2 e^{ik_2 a} - F i k_2 e^{ik_2 a} + C i k_2 e^{ik_2 a} = F i k_1 e^{ik_1 a}$$

$$\begin{aligned} &\Rightarrow 2C k_2 e^{ik_2 a} = F (k_1 + k_2) e^{ik_1 a} \\ &\Rightarrow C = \frac{1}{2} F \left( \frac{k_1 + k_2}{k_2} \right) e^{ik_1 a} e^{-ik_2 a}. \end{aligned}$$

Multiplying equation (2) by  $ik_2$  and solving for the term with the coefficient of  $C$ ,

$$C ik_2 e^{ik_2 a} = F ik_2 e^{ik_1 a} - D ik_2 e^{-ik_2 a}$$

and using this in equation (4),

$$\begin{aligned} F ik_2 e^{ik_1 a} - D ik_2 e^{-ik_2 a} - D ik_2 e^{-ik_2 a} &= F ik_1 e^{ik_1 a} \\ -2D k_2 e^{-ik_2 a} &= F (k_1 - k_2) e^{ik_1 a} \\ D &= \frac{1}{2} F \left( \frac{k_2 - k_1}{k_2} \right) e^{ik_1 a} e^{ik_2 a}. \end{aligned}$$

Substituting the relationships for  $C$  and  $D$  into equation (5) yields

$$\begin{aligned} 2A e^{-ik_1 a} &= \frac{1}{2} F \left( \frac{k_1 + k_2}{k_2} \right) \left( \frac{k_1 + k_2}{k_1} \right) e^{ik_1 a} e^{-2ik_2 a} + \frac{1}{2} F \left( \frac{k_2 - k_1}{k_2} \right) \left( \frac{k_1 - k_2}{k_1} \right) e^{ik_1 a} e^{2ik_2 a} \\ &= \frac{F}{2} e^{ik_1 a} \frac{(k_1^2 + 2k_1 k_2 + k_2^2)}{k_1 k_2} e^{-2ik_2 a} - \frac{F}{2} e^{ik_1 a} \frac{(k_1^2 - 2k_1 k_2 + k_2^2)}{k_1 k_2} e^{2ik_2 a} \\ &= \frac{F}{2k_1 k_2} e^{ik_1 a} \left[ k_1^2 e^{-2ik_2 a} + 2k_1 k_2 e^{-2ik_2 a} + k_2^2 e^{-2ik_2 a} \right. \\ &\quad \left. - k_1^2 e^{2ik_2 a} + 2k_1 k_2 e^{2ik_2 a} - k_2^2 e^{2ik_2 a} \right] \\ &= \frac{F}{2k_1 k_2} e^{ik_1 a} \left[ -k_1^2 (e^{2ik_2 a} - e^{-2ik_2 a}) + 2k_1 k_2 (e^{2ik_2 a} + e^{-2ik_2 a}) - k_2^2 (e^{2ik_2 a} - e^{-2ik_2 a}) \right] \\ &= \frac{F}{2k_1 k_2} e^{ik_1 a} \left[ -2ik_1^2 \sin(2k_2 a) + 4k_1 k_2 \cos(2k_2 a) - 2ik_2^2 \sin(2k_2 a) \right] \\ &= F e^{ik_1 a} \left[ 2 \cos(2k_2 a) - i \frac{(k_1^2 + k_2^2)}{k_1 k_2} \sin(2k_2 a) \right] \\ &\Rightarrow \frac{A e^{-ik_1 a}}{F e^{ik_1 a}} = \left[ \cos(2k_2 a) - \frac{i (k_1^2 + k_2^2)}{2 k_1 k_2} \sin(2k_2 a) \right]. \end{aligned}$$

$$\text{Since } \left| \frac{A e^{-ik_1 a}}{F e^{ik_1 a}} \right| = \left| \frac{A}{F} \right| = \frac{|A|}{|F|},$$

$$\begin{aligned} \frac{|A|^2}{|F|^2} &= \left| \cos(2k_2 a) - \frac{i (k_1^2 + k_2^2)}{2 k_1 k_2} \sin(2k_2 a) \right|^2 \\ &= \cos^2(2k_2 a) + \frac{1}{4} \left( \frac{k_1^2 + k_2^2}{k_1 k_2} \right)^2 \sin^2(2k_2 a). \end{aligned}$$

Adding zero in the form of  $\sin^2(2k_2 a) - \sin^2(2k_2 a)$ ,

$$\begin{aligned} \frac{|A|^2}{|F|^2} &= \cos^2(2k_2 a) + \sin^2(2k_2 a) - \sin^2(2k_2 a) + \frac{1}{4} \left( \frac{k_1^2 + k_2^2}{k_1 k_2} \right)^2 \sin^2(2k_2 a) \\ &= 1 + \left[ \frac{1}{4} \left( \frac{k_1^2 + k_2^2}{k_1 k_2} \right)^2 - 1 \right] \sin^2(2k_2 a). \end{aligned} \tag{6}$$

The expression in the square brackets reduces,

$$\frac{1}{4} \left( \frac{k_1^2 + k_2^2}{k_1 k_2} \right)^2 - 1 = \frac{k_1^4 + 2k_1^2 k_2^2 + k_2^4}{4k_1^2 k_2^2} - \frac{4k_1^2 k_2^2}{4k_1^2 k_2^2} = \frac{k_1^4 - 2k_1^2 k_2^2 + k_2^4}{4k_1^2 k_2^2} = \frac{1}{4} \left( \frac{k_1^2 - k_2^2}{k_1 k_2} \right)^2.$$

In terms of energy where  $k_1 = \sqrt{2mE}/\hbar$  and  $k_2 = \sqrt{2m(E - V_0)}/\hbar$ , this is

$$\frac{1}{4} \left( \frac{\frac{2m}{\hbar^2} E - \frac{2m}{\hbar^2} (E - V_0)}{\frac{2m}{\hbar^2} \sqrt{E} \sqrt{(E - V_0)}} \right)^2 = \frac{1}{4} \left( \frac{E - E + V_0}{\sqrt{E} \sqrt{(E - V_0)}} \right)^2 = \frac{V_0^2}{4E(E - V_0)}.$$

Using this in equation (6) and expressing the wave number in the argument of the sine in terms of energy, we arrive at the desired form,

$$\frac{|A|^2}{|F|^2} = T^{-1} = 1 + \frac{V_0^2}{4E(E - V_0)} \sin^2 \left( \frac{2a}{\hbar} \sqrt{2m(E - V_0)} \right).$$

12. (a) There are only two regions to consider, so the wave function is

$$\psi(x) = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1 x}, & \text{for } x < 0, \\ Ce^{ik_2 x}, & \text{for } x > 0, \end{cases}$$

where  $k_1 = \sqrt{2mE}/\hbar$  and  $k_2 = \sqrt{2m(E - (-V_0))}/\hbar = \sqrt{2m(E + V_0)}/\hbar$ , and the coefficient of a term like  $De^{-ik_2 x}$  must be zero for  $x > 0$  because it is the coefficient of an oppositely directed incident wave so is non-physical.

(b) The derivatives of the wave function are

$$\psi'(x) = \begin{cases} A ik_1 e^{ik_1 x} - B ik_1 e^{-ik_1 x}, & \text{for } x < 0, \\ C ik_2 e^{ik_2 x}, & \text{for } x > 0. \end{cases}$$

Continuity of  $\psi(x)$  at  $x = 0$  means  $A + B = C$  because the arguments of all exponentials are zero. Continuity of  $\psi'(x)$  at  $x = 0$  means

$$A ik_1 - B ik_1 = C ik_2.$$

Using  $C = A + B$  to eliminate  $C$ ,

$$\begin{aligned} A ik_1 - B ik_1 &= (A + B) ik_2 \\ &= A ik_2 + B ik_2 \\ \Rightarrow Ai(k_1 - k_2) &= Bi(k_1 + k_2) \\ \Rightarrow A(k_1 - k_2) &= B(k_1 + k_2). \end{aligned}$$

(c) The reflection coefficient is the ratio of the squares of the amplitudes of that portion reflected to that portion incident. Using the result of part (b),

$$\begin{aligned} A(k_1 - k_2) &= B(k_1 + k_2) \\ \Rightarrow \frac{B}{A} &= \frac{k_1 - k_2}{k_1 + k_2} \\ \Rightarrow \left| \frac{B}{A} \right|^2 &= \left( \frac{k_1 - k_2}{k_1 + k_2} \right)^2. \end{aligned}$$

Inserting values for the wave numbers, where  $k_1 = \sqrt{2mE}/\hbar$  and  $k_2 = \sqrt{2m(E + V_0)}/\hbar$ ,

$$\begin{aligned} \left| \frac{B}{A} \right|^2 &= \left( \frac{\sqrt{2mE}/\hbar - \sqrt{2m(E + V_0)}/\hbar}{\sqrt{2mE}/\hbar + \sqrt{2m(E + V_0)}/\hbar} \right)^2 \\ &= \left( \frac{\sqrt{E} - \sqrt{E + V_0}}{\sqrt{E} + \sqrt{E + V_0}} \right)^2 \\ &= \left( \frac{1 - \sqrt{1 + V_0/E}}{1 + \sqrt{1 + V_0/E}} \right)^2. \end{aligned}$$

If  $E = V_0/3$ , the ratio  $V_0/E = V_0/(V_0/3) = 3$ , and

$$\begin{aligned} \left| \frac{B}{A} \right|^2 &= \left( \frac{1 - \sqrt{1 + 3}}{1 + \sqrt{1 + 3}} \right)^2 = \left( \frac{1 - \sqrt{4}}{1 + \sqrt{4}} \right)^2 = \left( \frac{1 - 2}{1 + 2} \right)^2 = \left( \frac{-1}{3} \right)^2 \\ &\Rightarrow \left| \frac{B}{A} \right|^2 = R = \frac{1}{9} \quad \Rightarrow \quad T = \frac{8}{9}. \end{aligned}$$

If  $E = V_0/8$ , the ratio  $V_0/E = V_0/(V_0/8) = 8$ , and

$$\begin{aligned} \left| \frac{B}{A} \right|^2 &= \left( \frac{1 - \sqrt{1 + 8}}{1 + \sqrt{1 + 8}} \right)^2 = \left( \frac{1 - \sqrt{9}}{1 + \sqrt{9}} \right)^2 = \left( \frac{1 - 3}{1 + 3} \right)^2 = \left( \frac{-2}{4} \right)^2 \\ &\Rightarrow \left| \frac{B}{A} \right|^2 = R = \frac{1}{4} \quad \Rightarrow \quad T = \frac{3}{4}. \end{aligned}$$

13. (a) The wave numbers are comparable to those from problem 12 where  $k_1 = \sqrt{2mE}/\hbar$  and  $k_2 = \sqrt{2m(E - (-V_0))}/\hbar = \sqrt{2m(E + V_0)}/\hbar$ . The solution to this problem is procedurally the same as problems 3 and 10 with the exception of the wave numbers. The differences are  $k$  in problem 3 is replaced by  $k_1$  and  $\kappa$  in problem 3 is replaced with  $ik_2$ , and a  $\sin$  emerges instead of a  $\sinh$ . The first substantial difference is when wave numbers are replaced by energies in part (d). The comparable circumstance for the square well is

$$\frac{|A|^2}{|F|^2} = 1 + \frac{(k_1^2 - k_2^2)^2}{4k_1^2 k_2^2} \sin^2(2k_2 a)$$

so substituting the appropriate wave numbers,

$$\begin{aligned} \frac{|A|^2}{|F|^2} &= 1 + \frac{\left( \frac{2m}{\hbar^2} E - \frac{2m}{\hbar^2} (E + V_0) \right)^2}{4 \left( \frac{2m}{\hbar^2} E \right) \left( \frac{2m}{\hbar^2} (E + V_0) \right)} \sin^2 \left( \frac{2a}{\hbar} \sqrt{2m(E + V_0)} \right) \\ &= 1 + \frac{\frac{4m^2}{\hbar^4} (E - E - V_0)^2}{\frac{4m^2}{\hbar^4} 4E (E + V_0)} \sin^2 \left( \frac{2a}{\hbar} \sqrt{2m(E + V_0)} \right) \\ &\Rightarrow \frac{|A|^2}{|F|^2} = T^{-1} = 1 + \frac{V_0^2}{4E(E + V_0)} \sin^2 \left( \frac{2a}{\hbar} \sqrt{2m(E + V_0)} \right). \end{aligned}$$

(b)  $V_0 = 0 \Rightarrow a = 0$ . If  $a = 0$ , the  $\sin^2$  term is zero, so  $T = 1$  when  $V_0 = 0$ .

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15. The result of problem 4 for  $E = V_0$  is

$$\frac{1}{T} = 1 + \frac{2mE}{\hbar^2} a^2.$$

The de Broglie wavelength is

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \Rightarrow \sqrt{2mE} = \frac{h}{\lambda} \Rightarrow E = \frac{h^2}{2m\lambda^2},$$

so the reciprocal of the transmission coefficient is

$$\frac{1}{T} = 1 + \frac{2m \left( \frac{h^2}{2m\lambda^2} \right)}{\left( \frac{h}{2\pi} \right)^2} a^2 = 1 + \frac{4\pi^2 a^2}{\lambda^2}$$

$$\Rightarrow \frac{4\pi^2 a^2}{\lambda^2} = \frac{1}{T} - 1 \Rightarrow 4\pi^2 a^2 = \lambda^2 \left( \frac{1}{T} - 1 \right) \Rightarrow a = \frac{\lambda}{2\pi} \left( \frac{1}{T} - 1 \right)^{1/2}.$$

Remember  $2a$  is the width of the barrier, so

$$2a = \frac{\lambda}{\pi} \left( \frac{1}{T} - 1 \right)^{1/2}.$$

This is barrier width in terms of wavelength and transmission coefficient, and the graph is at the right. It can be interpreted as the barrier width in terms of wavelength for a given value of the transmission coefficient. A numerical value is

$$2a = \frac{\lambda}{\pi} \left( \frac{1}{0.1} - 1 \right)^{1/2} = \frac{\lambda}{\pi} (10 - 1)^{1/2} = \frac{\lambda}{\pi} (9)^{1/2} = 0.955\lambda$$

for 10% transmission. Notice that this is less than one particle wavelength. The others are calculated similarly, using  $T = 0.01$ ,  $0.001$ , and  $0.0001$  respectively, so the four requested numerical values are

% transmission	$T$	$2a$
10%	0.1	$0.955\lambda$
1%	0.01	$3.167\lambda$
0.1%	0.001	$10.061\lambda$
0.01%	0.0001	$31.829\lambda$

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