PROBLEMS

7.1 The Square Barrier

1. A particle incident on the potential step of Example 7.4 with a certain energy $E < U$ is described by the wave

$$\psi(x) = \tfrac{1}{2}\{(1+i)e^{ikx} + (1-i)e^{-ikx}\} \qquad \text{for } x \le 0$$
$$\psi(x) = e^{-kx} \qquad \text{for } x \ge 0$$

(a) Verify by direct calculation that the reflection coefficient is unity in this case. (b) How must k be related to E in order for $\psi(x)$ to solve Schrödinger's equation in the region to the left of the step ($x \le 0$)? to the right of the step ($x > 0$)? What does this say about the ratio E/U? (c) Evaluate the penetration depth $\delta = 1/k$ for 10 MeV protons incident on this step.

2. Consider the step potential of Example 7.4 in the case where $E > U$. (a) Examine the Schrödinger equation to the left of the step to find the form of the solution in the range $x < 0$. Do the same to the right of the step to obtain the solution form for $x > 0$. Complete the solution by enforcing whatever boundary and matching conditions may be necessary. (b) Obtain an expression for the reflection coefficient R in this case, and show that it can be written in the form

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}$$

where k_1 and k_2 are wavenumbers for the incident and transmitted waves, respectively. Also write an expression for the transmission factor T using the sum rule obeyed by these coefficients. (c) Evaluate R and T in the limiting cases of $E \to U$ and $E \to \infty$. Are the results sensible? Explain. (This situation is analogous to the partial reflection and transmission of light striking an interface separating two different media.)

3. Use the results of the preceding problem to calculate the fraction of 25-MeV protons reflected and the fraction transmitted by a 20-MeV step. How do your answers change if the protons are replaced by electrons?

4. A 0.100-mA electron beam with kinetic energy 54.0 eV enters a sharply defined region of *lower* potential where the kinetic energy of the electrons is increased by 10.0 eV. What current is reflected at the boundary? (This simulates electron scattering at normal incidence from a metal surface, as in the Davisson–Germer experiment.)

5. (a) Tunneling of particles through barriers that are high or wide (or both) is very unlikely. Show that for a square barrier with

$$\frac{2mUL^2}{\hbar^2} >> 1$$

and particle energies well below the top of the barrier ($E << U$) the probability for transmission is approximately

$$P \approx 16\,\frac{E}{U}\,e^{-2[\sqrt{2m(U-E)}/\hbar]L}$$

(The combination UL^2 is sometimes referred to as the barrier *strength.*) (b) Give numerical estimates for the exponential factor in P for each of the following cases: (1) an electron with $U - E = 0.01$ eV and $L = 0.1$ nm; (2) an electron with $U - E = 1$ eV and $L = 0.1$ nm; (3) an α particle ($m = 6.7 \times 10^{-27}$ kg) with $U - E = 10^6$ eV and $L = 10^{-15}$ m; and (4) a bowling ball ($m = 8$ kg) with $U - E = 1$ J and $L = 2$ cm (this corresponds to the ball's getting past a barrier 2 cm wide and too high for the ball to slide over).

6. A beam of electrons is incident on a barrier 5 eV high and 1 nm wide. Write a simple computer program to find what energy the electrons should have if 0.1% of them are to get through the barrier.

7. Starting from the joining conditions, Equations 7.8, obtain the result for the transmission coefficient of a square barrier given in Equation 7.9 (valid when the particle has insufficient energy to penetrate the barrier classically: $E < U$).

8. Use the Java applet available at our companion Web site (http://info.brookscole.com/mp3e QMTools Simulations → Problem 7.8) to investigate the scattering of electrons from a square barrier 1.00 Å thick and 10.0 eV high, in the case where the electron energy is equal to the barrier height, $E = U$. What is the functional form of the wave in the barrier region? Determine the transmission coefficient at this energy, and compare your result with the prediction of Equation 7.9. What does classical physics predict for the probability of transmission in this case?

9. Use the Java applet referenced in the preceding problem to obtain transmission and reflection coefficients for a 5.00-eV electron incident on a square barrier that is 1.00 Å thick and 10.0 eV high. Verify the sum rule, Equation 7.5, and compare your result for $T(E)$ with the prediction of Equation 7.9. What must the barrier thickness be to transmit 5.00-eV *protons* with the same probability?

10. *Scattering resonances.* Use the Java applet available at our companion Web site (http://info.brookscole.com/mp3e QMTools Simulations → Problem 7.10) to locate the two lowest energies E giving rise to perfect transmission for electrons scattering from a square barrier of width 1.00 Å and height 10.0 eV (look for zero-amplitude reflections while varying E). For each energy use the "Trace" feature to estimate the electron wavelength λ in the barrier. (*Hint*: Zoom in for a close-up view of the barrier waveform and greater accuracy.) Compare λ with the barrier width L and dis-

cuss your findings in terms of the interference of waves reflected from the leading and trailing edges of the barrier (see Example 7.3).

11. *The Ramsauer–Townsend effect*. Consider the scattering of particles from the potential well shown in Figure P7.11. (a) Explain why the waves reflected from the well edges $x = 0$ and $x = L$ will cancel completely if $2L = \lambda_2$, where λ_2 is the de Broglie wavelength of the particle in region 2. (b) Write expressions for the wavefunctions in regions 1, 2, and 3. Impose the necessary continuity restrictions on Ψ and $\partial\Psi/\partial x$ to show explicitly that $2L = \lambda_2$ leads to no reflected wave in region 1. [This is a crude model for the Ramsauer–Townsend effect observed in the collisions of slow electrons with noble gas atoms like argon, krypton, and xenon. Electrons with just the right energy are diffracted around these atoms as if there were no obstacle in their path (perfect transmission). The effect is peculiar to the noble gases because their closed-shell configurations produce atoms with abrupt outer boundaries.]

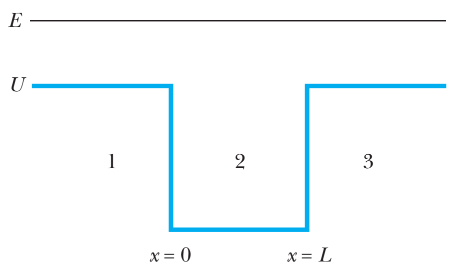

Figure P7.11

12. A potential model of interest for its simplicity is the *delta well*. The delta well may be thought of as a square well of width L and depth S/L in the limit $L \to 0$ (Fig. P7.12). The limit is such that S, the product of the well depth with its width, remains fixed at a finite value known as the well strength. The effect of a delta well is to introduce a discontinuity in the slope of the wavefunction at the well site, although the wave itself remains continuous here. In particular, it can be shown that

$$\left.\frac{d\psi}{dx}\right|_{0+} - \left.\frac{d\psi}{dx}\right|_{0-} = -\frac{2mS}{\hbar^2}\psi(0)$$

for a delta well of strength S situated at $x = 0$. (a) Solve Schrödinger's equation on both sides of the well ($x < 0$ and $x > 0$) for the case where particles are incident from the left with energy $E > 0$. Note that in these regions the particles are free, so that $U(x) = 0$. (b) Enforce the continuity of ψ and the slope condition at $x = 0$. Solve the resulting equations to obtain the transmission coefficient T as a function of particle energy E. Sketch $T(E)$ for $E \geq 0$. (c) If we allow E to be negative, we find that $T(E)$ diverges for some particular energy E_0. Find this value E_0. (As it happens, E_0 is the energy of a *bound state* in the delta well. The calculation illustrates a general technique, in which bound states are sought among the singularities of the scattering coefficients for a potential well of arbitrary shape.) (d) What fraction of the particles incident on the well with energy $E = |E_0|$ is transmitted and what fraction is reflected?

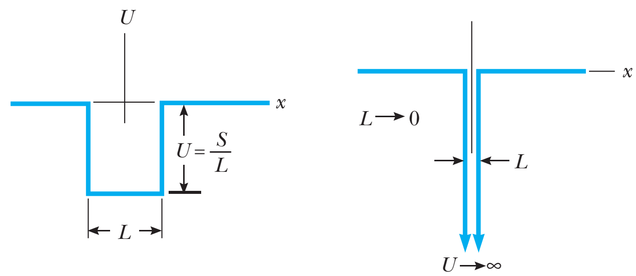

Figure P7.12

13. Obtain directly an expression for the reflection coefficient $R(E)$ for the delta well of Problem 12, and verify the sum rule

$$R(E) + T(E) = 1$$

for all particle energies $E > 0$.

14. Keeping constant speed 0.8 m/s, a marble rolls back and forth inside a shoebox. Make an order-of-magnitude estimate of the probability of its escaping through the wall of the box by quantum tunneling. State the quantities you take as data and the values you measure or estimate for them.

7.2 Barrier Penetration

15. A barrier of arbitrary shape can be approximated as a succession of square barriers, as shown in Figure P7.15. Write the transmission coefficient for this barrier using the result of Equation 7.9 for each of the individual barriers, assuming the transmitted wave intensity for one becomes the incident wave intensity for the barrier immediately following it in the series. Show that the form of Equation 7.10 is recovered in the case where $E < U$ and $\alpha L \gg 1$.

16. Consider an α particle confined to a thorium nucleus. Model the nuclear potential as a semi-infinite square well with an infinitely high wall at $r = 0$ and a wall of height 30.0 MeV at the nuclear radius $R = 9.00$ fm. Use the iterative method described in Example 6.8 to estimate the smallest values of energy and velocity permitted for the α particle. What conclusion can you draw from the fact that the *ejected* α is observed to have a kinetic energy of 4.05 MeV?

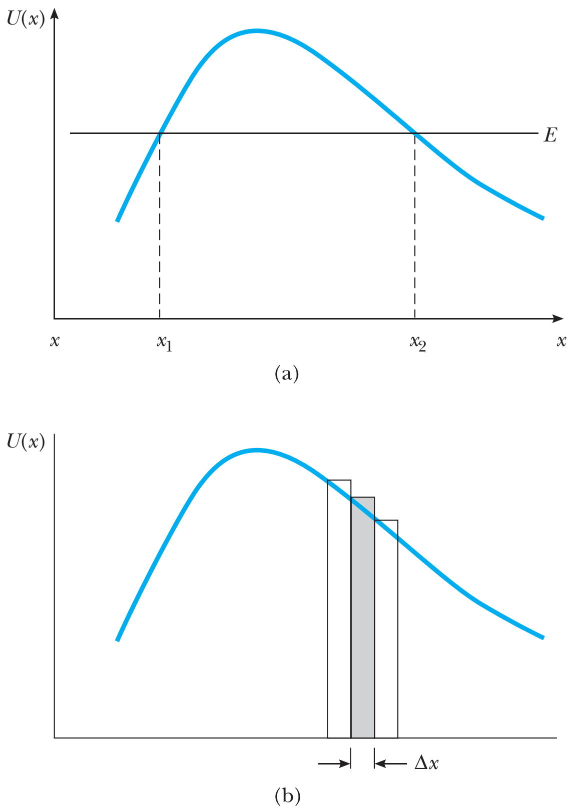

Figure P7.15

17. The attempt frequency of an α particle to escape the nucleus is the number of times per second it collides with the nuclear barrier. Estimate this collision frequency in the tunneling model for the α decay of thorium, assuming the α behaves like a true particle inside the nucleus with *total* energy equal to the observed kinetic energy of decay. The daughter nucleus for this case (radium) has $Z = 88$ and a radius of 9.00 fm. Take for the overall nuclear barrier 30.0 MeV, measured from the bottom of the nuclear well to the top of the Coulomb barrier (see Fig. 7.8).
18. Verify the claim of Section 7.2 that the electrons of a metal collide with the surface at a rate of about 10^{30} per second per square centimeter. Do this by estimating the collision frequency of electrons in a 1.00-cm cube of copper metal with one face of the cube surface. Assume that each copper atom contributes one conduction electron to the metal (the chemical valence of copper is $+1$) and that these conduction electrons move freely with kinetic energy equal to 7.00 eV. In fact, not all the electrons have this energy; see Chapter 10.
19. *Resonant tunneling.* Heterostructures formed from layered semiconductors have characteristics important to many modern electronic devices. Here, we use computer simulation to study tunneling in a three-layer gallium arsenide/gallium aluminum arsenide (GaAs–$Ga_{1-x}Al_xAs$) sandwich. The GaAs layer constitutes a potential well between two confining barriers formed by the $Ga_{1-x}Al_xAs$ layers. Unusually large transmission (resonant tunneling) through the device occurs when the energy of the incident electron coincides with that of a bound state in the central well. The Java applet simulating this device can be found at http://info.brookscole.com/mp3e QMTools Simulations → Problem 7.19. The barriers are 0.25 eV high and 5.0 nm wide, with a gap of equal width separating them. Note that electrons in these materials behave like free electrons with an effective mass $m^* = 0.067m_e$, only a fraction of the free electron value. Starting from $E = 0$, gradually increase the electron energy to find the lowest value for peak transmission. Investigate the width of the resonance by varying the electron energy further until $T(E)$ falls to half of its peak value. (In practice, the incident electron energy is fixed and the device is "tuned" to resonance by applying a suitable bias voltage that alters the bound-state energies of the central well.)
20. *Ammonia inversion.* Inversion of the ammonia molecule can be simulated using the Java applet available at our companion Web site (http://info.brookscole.com/mp3e QMTools Simulations → Problem 7.20) The potential energy is the double oscillator of Equation 7.15 with parameter values chosen to model the nitrogen atom in NH_3 (as discussed in the text) and a reduced mass of 2.47 u for the atom in this environment. (a) Find and display the two lowest-lying stationary states of the nitrogen atom in the ammonia molecule. Describe the appearance of these waveforms (symmetry, number of nodes, and so on). (b) Construct an initial (nonstationary) state for the atom by mixing together these two stationary waves with equal amplitude. Describe this state. What does it imply for the location of the atom initially? (c) Explore the time evolution of the state constructed in (b). Verify that the atom flip-flops between the two equilibrium positions and determine the "flopping" frequency. Multiplying the flopping frequency by Planck's constant gives a characteristic energy for this process. How does this characteristic energy compare to the energy separation of the stationary states? Explain (see Problem 6.38).