1 Scattering and Barrier Penetration in 1-D

1.1 Governing Equation

We wish to examine the interaction of a free particle with a potential in one dimension. To do this we need the scaled, time-independent, one-dimensional Schrödinger equation for the wavefunction ψ:

$$\frac{\partial^2 \psi}{\partial x^2} + 2(\epsilon - u)\psi = 0, \tag{1}$$

where $\epsilon = mL^2E/\hbar^2$, $u = mL^2U/\hbar^2$, and L is the assumed x scaling factor. Notice that since the second derivative of ψ is the curvature of $\psi(x)$, this equation has an oscillatory character if $\epsilon > u$ and an exponential character if $\epsilon < u$.

The free wave solution to equation (1), i. e., that solution which applies where $u = 0$, is simply

$$\psi = \psi_L \exp(-ik_f x) + \psi_R \exp(ik_f x), \tag{2}$$

where the wavenumber k_f is given by

$$k_f = (2\epsilon)^{1/2}. \tag{3}$$

The amplitude for the left-moving wave is ψ_L and the amplitude for the right-moving wave is ψ_R.

1.2 Step Function Potential

The simplest potential we can consider is a step function, as shown in figure 1. In this example the potential is zero for $x > 0$ and is a nonzero constant value, u, for $x < 0$. The solution for $x > 0$ consists of incident and reflected components, while for $x < 0$ a single transmitted component moving in the incident direction, i. e., to the left, is found. The transmitted component has a nondimensional wavenumber equal to $k_t = [2(\epsilon - u)]^{1/2}$ for $u < \epsilon$ and $k_t = i[2(u - \epsilon)]^{1/2}$ for $u > \epsilon$. The sign of the latter expression is chosen so that $\exp(-ik_t x)$ decays exponentially to the left. The wavefunction thus has the form

$$\psi = \begin{cases} I \exp(-ik_f x) + R \exp(ik_f x) & , \ x > 0 \\ T \exp(-ik_t x) & , \ x < 0 \end{cases} . \tag{4}$$

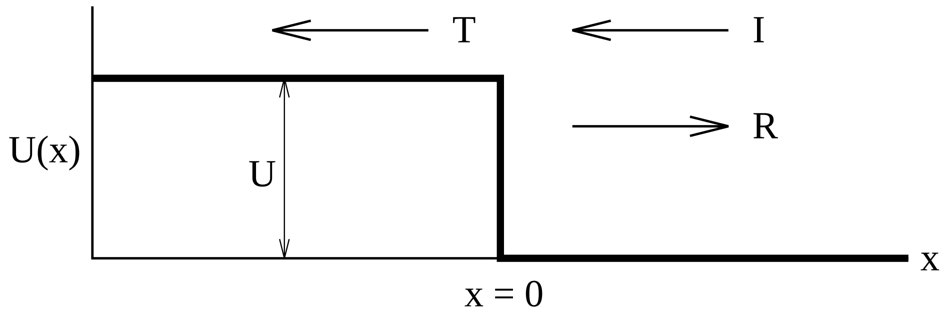

Figure 1: Defining sketch for the step function potential.

Applying the connecting conditions at $x = 0$, namely continuity of ψ and $\partial\psi/\partial x$, we find relationships between I, R, and T:

$$I + R = T, \tag{5}$$

$$-I + R = -(k_t/k_f)T. \tag{6}$$

The resulting solutions for the transmitted and reflected amplitudes are

$$\frac{T}{I} = \frac{2}{1 + k_t/k_f}, \qquad \frac{R}{I} = \frac{1 - k_t/k_f}{1 + k_t/k_f}. \tag{7}$$

It is easy to show that the ratio of the minimum and maximum values of $|\psi|$ for $x > 0$ is

$$\eta \equiv \frac{|\psi|_{min}}{|\psi|_{max}} = \frac{1 - |R/I|}{1 + |R/I|}. \tag{8}$$

Notice that there are three distinct cases, $u < 0$, $0 < u < \epsilon$ and $u > \epsilon$:

$$\eta = \left\{ \begin{array}{ll} k_f/k_t = (\epsilon/(\epsilon - u))^{1/2} & , \ u < 0 \\ k_t/k_f = ((\epsilon - u)/\epsilon)^{1/2} & , \ 0 < u < \epsilon \\ 0 & , \ u > \epsilon \end{array} \right. . \tag{9}$$

For the first two cases there is partial reflection and a partial standing wave for $x > 0$. The magnitude of η is inversely related to the strength of the reflected wave. As u approaches $+\epsilon$ or $-\infty$, the reflection becomes total, resulting in $\eta = 0$. For $u > \epsilon$ the region $x < 0$ is classically forbidden to the particle, and only an evanescent, or exponentially decaying wave exists for $x < 0$.

Quantum mechanics thus differs from classical mechanics in that there is a small but finite probability of finding a particle in a region that is classically forbidden on energy grounds. This can be related to the uncertainty principle: The part of the forbidden region accessible to the particle is quite close to the $x = 0$ interface between the two regions, so localizing the particle to within this accessible region gives it an uncertainty in the momentum. The energy in turn is uncertain to the degree necessary to avoid a violation of energy conservation.

1.3 Arbitrary Potential

For a potential $u(x)$ that is arbitrary within some distance D of $x = 0$, but is known to be zero (or very close to zero) outside this region, equation (9) can be used to determine the probabilities for reflection, P_r, and transmission, P_t, of an incident particle as long as (9) is evaluated where $x > D$. It is easy to show in this case that

$$P_r = \left(\frac{1-\eta}{1+\eta}\right)^2 \tag{10}$$

and

$$P_t = 1 - P_r. \tag{11}$$

Equation (1) can be solved numerically by rewriting it as two coupled first order equations,

$$\frac{\partial\psi}{\partial x} = \chi \tag{12}$$

and

$$\frac{\partial\chi}{\partial x} = 2(u - \epsilon)\psi. \tag{13}$$

If we assume that particles are coming in from the right, then the solution to the left of the potential has only a leftward-moving component, as discussed above. In the region where $u = 0$, the spatial dependence of this solution is $\exp[-i(2\epsilon)^{1/2}x]$. Equation (12) shows that $\chi = -i(2\epsilon)^{1/2}\psi$ in this region. Thus equations (12) and (13) can be jointly solved by specifying initial values at the left end of the domain and integrating numerically to the right in x.

The RLaB demonstration *scatter1_demo.r* uses these equations to compute ψ, P_r, and P_t for a variety of potentials.

1.4 Barrier Penetration

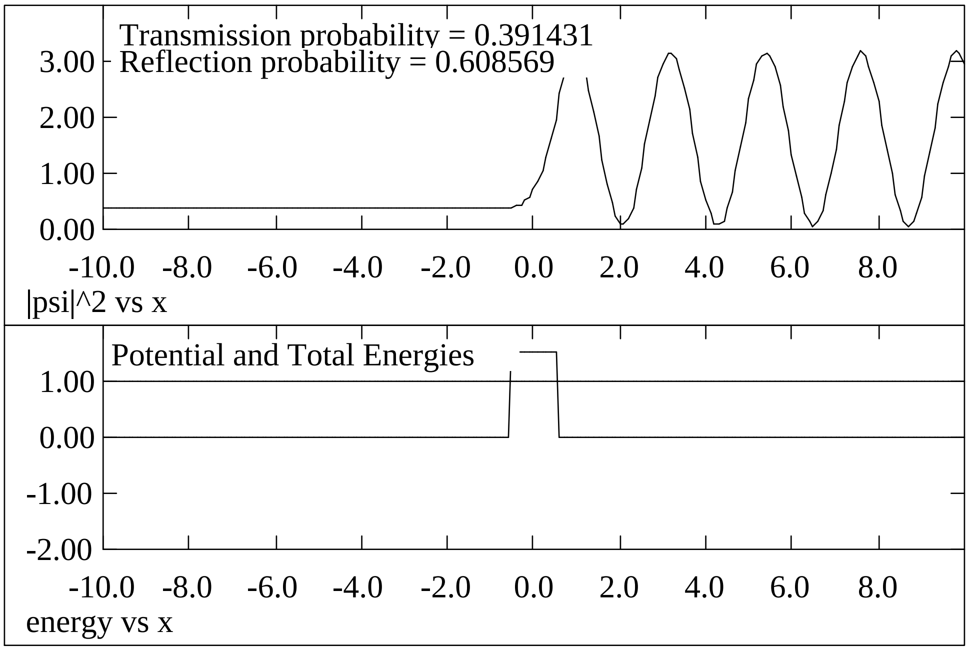

Figure 2: Example of barrier penetration. Upper plot shows $|\psi|^2$ for a particle entering from the right. Lower plot shows the energy of the particle (dashed line) and the potential energy function (filled region). This plot was made using the RLaB demonstration program *scatter1_demo.r*.

Since particles in quantum mechanics can potentially be found in regions that are classically forbidden by energy considerations, this raises the possibility of particles actually passing through narrow forbidden regions. Figure 2 shows an example of such *barrier penetration*, calculated using *scatter1_demo.r*. Notice how the absolute square of the wavefunction decays exponentially to the left in the barrier region where the potential energy is 1.5 times the total energy. As discussed above, the region to the right of the barrier exhibits a standing wave, represented by the oscillations in $|\psi|^2$. The probability of the particle penetrating this barrier is approximately 0.39.

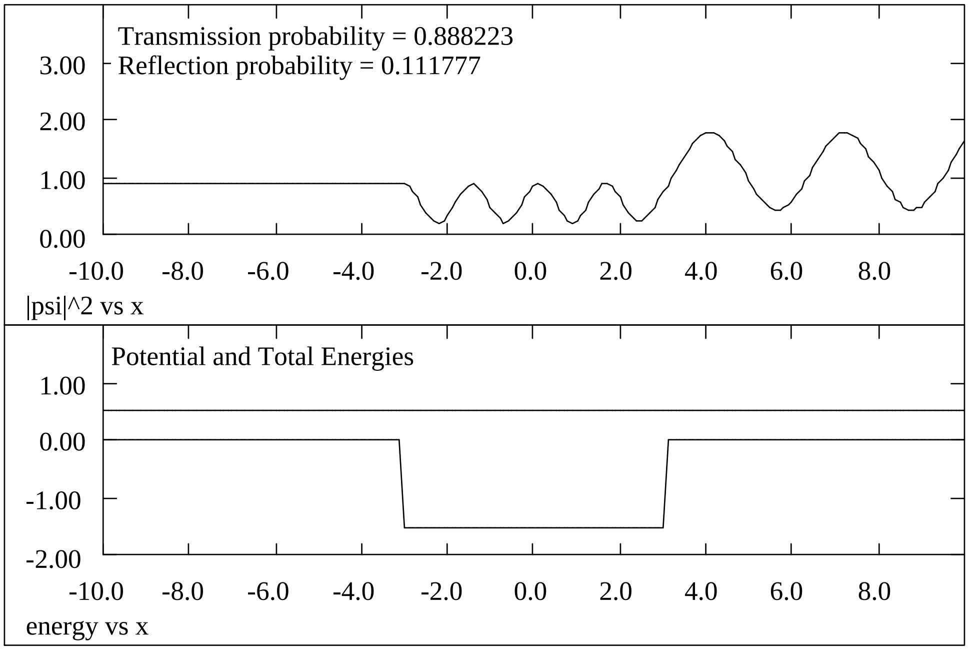

Figure 3: Passage of a wave through a region of negative potential energy. The total dimensionless energy is 0.5.

1.5 Negative Potential Energies

Figure 3 shows the passage of a wave through a region of negative potential energy. Even though the potential is not a barrier in a classical sense, the wave is partially reflected. Figure 4 shows the reflection coefficient as a function of energy for the potential shown in figure 3. Particularly large values of the reflection coefficient are seen for small total energies. This occurs because the ratio of the kinetic energies inside and outside of the potential well is then large. Note also that the reflection coefficient oscillates with energy, with certain energies resulting in zero reflection. This is reminiscent of the destructive interference that occurs between reflections from the front and back surfaces of a thin film when light passes through it.

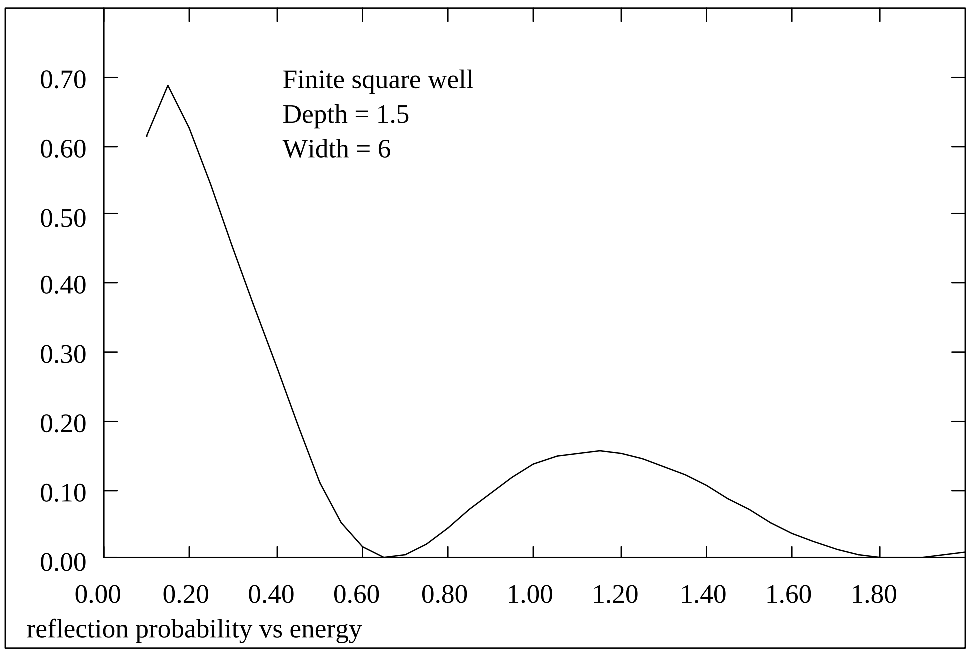

Figure 4: Reflection coefficient as a function of energy for the potential well shown in figure 3.