

Potential Step: Griffiths Problem 2.33

Prelude: Note that the time-independent Schrödinger equation in one dimension can be written as

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2} (E - V(x)) \psi(x). \quad (1)$$

This second-order differential equation is difficult to solve even for simple potentials encountered in classical mechanics, e.g., a charged particle in a constant electric field, $V(x) = -qEx$ which leads to a constant force (i.e., constant acceleration, $x = x_0 + v_0t + (1/2)at^2$ and all that!) or the simple harmonic oscillator, $V(x) = (1/2)m\omega^2x^2$. In quantum mechanics former leads to what are known as *Airy functions* and the latter involve *Hermite polynomials*.

The simplest examples which nevertheless illustrate some very interesting quantum mechanical phenomena are those in which the potential $V(x)$ is *piecewise constant*. In each of the regions in which the potentials is a constant, say $V = V_0$, the solution is clearly a combination of exponentials:

(i) If $E > V_0$ then we write the Schrödinger equation as

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2} (E - V_0) \psi(x) = -k^2 \psi(x).$$

In the preceding we have defined $\boxed{\frac{\hbar^2 k^2}{2m} = E - V_0}$. This equation determines the wavevector k given the energy and the potential. The solution is oscillatory: a linear combination e^{ikx} and e^{-ikx} which represent free-particle solutions moving to the right and to the left respectively. Note that k is the wavevector (assumed to be the positive root) and by the de Broglie relation the momentum $p = \hbar k$. Check that e^{ikx} is an eigenfunction of the momentum operator. The kinetic energy of the particle is $\frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$. The equation which determines the wavevector k simply states that the kinetic energy plus the potential energy equals the total energy E .

(ii) If $E < V_0$ in a region which the potential is a constant and equal to V_0 then we can write

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2} (V_0 - E) \psi(x) = \kappa^2 \psi(x).$$

where we have defined $\boxed{\frac{\hbar^2 \kappa^2}{2m} = V_0 - E}$. This equation determines the imaginary

wavevector κ given the energy and the potential. The solution is a linear combination of real exponentials, $e^{\kappa x}$ and $e^{-\kappa x}$. These decay for large negative and positive values of x respectively. In this region $V_0 > E$, i.e., the kinetic energy is negative and this region is said to be *classically forbidden*.

The solutions in regions with different (constant) potential values must be matched by using the continuity of ψ and $d\psi/dx$ on the two sides of a boundary where there is a (finite) discontinuous change in the value of the potential. Also we impose the condition that the wavefunction is not increasing in magnitude as $|x|$ becomes large.

The above considerations are important and will be employed in many examples.

Consider a potential step described by¹

$$V(x) = V_0 \text{ for } x > 0 \text{ and } V(x) = 0 \text{ for } x < 0. \quad (2)$$

We will first consider $E > V_0$ and denote the region of negative x by I and positive x by II and the corresponding wavefunctions $\psi_I(x)$ and $\psi_{II}(x)$ respectively. The Schrödinger equation reads

$$\frac{d^2\psi_I}{dx^2} = -k^2 \psi_I \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}} \quad (3)$$

$$\frac{d^2\psi_{II}}{dx^2} = -q^2 \psi_{II} \quad \text{where } q = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}. \quad (4)$$

The solutions are simple and are linear combinations of oscillating exponentials. Recall that if $\psi = \exp(\pm ikx)$, the expectation value of the momentum is $\pm\hbar k$ yielding particles moving to the right and left respectively. We will consider the case where there is no particle incident from the right (moving to the left), i.e., from region II. So we write

$$\psi_I(x) = e^{ikx} + r e^{-ikx} \quad x < 0 \quad (5)$$

$$\psi_{II}(x) = t e^{iqx} \quad x > 0 \quad (6)$$

where we have set the coefficient of the incident wave to be 1 for mathematical simplicity. (Note again that e^{ikx} is traveling to the right and is thus incident on the

¹This can be written more compactly as $V(x) = V_0 \theta(x)$ where $\theta(x)$ is the step function, equal to 1 for $x > 0$ and 0 for $x < 0$. It is sometimes called the Heaviside step function.

potential discontinuity) and r and t are the coefficients (amplitudes) of the reflected and transmitted waves respectively. The unknown quantities r and t (these can be complex!) are determined by using the continuity of ψ and $d\psi/dx$ (denoted by ψ') at $x = 0$. Matching boundary conditions we have

$$\psi_I(x=0) : \quad 1 + r = t \quad : \psi_{II}(x=0) \quad (7)$$

$$\psi'_I(x=0) : \quad ik(1 - r) = iqt \quad : \psi'_{II}(x=0) \quad (8)$$

which can be solved to obtain

$$r = \frac{k - q}{k + q} \quad (9)$$

$$t = \frac{2k}{k + q} \quad (10)$$

Let us make sure we understand this result. Classically, a particle incident on such a potential with $E > V_0$ will go across the potential step traveling with a lower speed in II (There is a force acting just at $x = 0$ since the force is the negative derivative of the potential and this force slows down the particle.) In quantum mechanics the particle has some probability (in an ensemble sense) to be reflected even though its energy is higher than the barrier. One way to quantify this is to calculate the current density incident on the step and determine what fraction of it is reflected and what fraction is transmitted.

Given the wave functions in the two regions it is simple to compute the current density in each region. Recall that

$$j = \frac{\hbar}{2im} \left[\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right] = \frac{\hbar}{m} \text{Im} \left[\psi^* \frac{d\psi(x)}{dx} \right].$$

Substituting the expressions for the wave functions in the two regions we find

$$j_I(x) = \frac{\hbar k}{m} (1 - |r|^2) \quad (11)$$

$$j_{II}(x) = \frac{\hbar q}{m} |t|^2 \quad (12)$$

Note that the (probability) current (density) in region I is the incident current density, j_{inc} , given by $\boxed{j_{inc} = \hbar k/m}$ minus the reflected current density, j_{ref} whose magnitude is given by $\boxed{|j_{ref}| = (\hbar k/m)|r|^2}$. The transmitted current density is similarly

$j_{tran} = (\hbar q/m)t^2$. The reflection and transmission coefficients are defined to be the ratio of the reflected current density to the incident current density and transmitted current to the incident current respectively:

$$R \equiv \frac{j_{ref}}{j_{inc}} \quad \text{and} \quad T \equiv \frac{j_{tran}}{j_{inc}} \quad (13)$$

Note that since we are dividing by the incident current density our choice of 1 for the coefficient of e^{ikx} loses no generality: If we had called it A , both r and t would be multiplied by A and it would disappear from R and T . Therefore, we obtain

$$R = \frac{(k - q)^2}{(k + q)^2} \quad \text{and} \quad T = \frac{4kq}{(k + q)^2} \quad (14)$$

You can check that

$$R + T = 1 \quad \text{i.e.,} \quad j_{inc} = j_{ref} + j_{tran} \quad (15)$$

i.e., the incident wave is partially reflected and the rest is transmitted showing conservation of particle number.

We find that the reflection coefficient is finite. Classically a particle is transmitted completely with only a diminution in velocity. Note that classically light waves are reflected at the boundary between two media in which the velocities are different, i.e., with different refractive indices. The quantum mechanical particle behaves like a wave. If you look up Griffiths' other book on electrodynamics (Chapter 8) you will find the reflection coefficient for light transmitted normally across a planar interface between two media:

$$r = \frac{(n_1 - n_2)^2}{(n_1 + n_2)^2}$$

where the refractive indices of the two media are $n_1 = c/v_1$ and $n_2 = c/v_2$ where v_i is the speed of light in medium i . Thus the reflection coefficient can be written as $(v_1 - v_2)^2/(v_1 + v_2)^2$ which should be compared with our result for a quantum mechanical particle. Convince yourself that it is the same. So as long as we accept the notion of the quantum mechanical particle behaving as a wave its behavior becomes somewhat more comprehensible.

For $E < V_0$, we have an exponentially decaying wave function for $x > 0$. So the wave functions in the two regions are

$$\begin{aligned}\psi_I(x) &= e^{ikx} + r e^{-ikx} \text{ for } x < 0 \\ \psi_{II}(x) &= A e^{-\kappa x} \text{ where } \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \text{ for } x > 0.\end{aligned}\quad (16)$$

The exponentially increasing solution has been discarded because it is unphysical (the particle is more and more likely to be found at larger and larger x and ψ will not be normalizable.) Continuity of the wave function and its derivative yield

$$1 + r = A \text{ and } ik(1 - r) = -A\kappa.$$

This yields

$$\frac{1 - r}{1 + r} = i \frac{\kappa}{k} \Rightarrow r = \frac{k - i\kappa}{k + i\kappa}.$$

Since k and κ are real $|r|^2 = 1$. Once more with emphasis, the numerator and denominator are complex conjugates of each other and hence both have the same length or modulus. The reflection coefficient is $|r|^2 = 1$. Since the sum of the reflection and transmission coefficients must be unity the transmission coefficient vanishes. Another way of seeing this is to observe that the transmitted current vanishes which follows from the fact that the wave function is real. One can write the reflected amplitude r as a phase factor since its magnitude is 1:

$$r = e^{-2i\delta} \text{ where } \tan \delta = \frac{\kappa}{k} = \sqrt{\frac{V_0}{E} - 1}.$$

As The incident wave is reflected with no change in the current but with a phase shift.