Potential Step

Consider a potential step described by[1]

$$V(x) = V_0 \text{ for } x > 0 \quad \text{and} \quad V(x) = 0 \text{ for } x < 0. \tag{1}$$

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

$$\frac{d^2\psi_I}{dx^2} = -k^2\,\psi_I \quad \text{where} \quad k = \sqrt{\frac{2mE}{\hbar^2}} \tag{2}$$

$$\frac{d^2\psi_{II}}{dx^2} = -q^2\,\psi_{II} \quad \text{where} \quad q = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} \;. \tag{3}$$

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 and left respectively. Imagine performing an experiment in which we fire particles with energy E from the left only; i.e., there are no particles incident from the right. The particles will be scattered by the potential and yield a part transmitted to $x > 0$ and another reflected back to $x < 0$. Since there are no particles incident from the right (moving to the left), the term e^{-iqx} will not be present in region II. So we write

$$\psi_{II}(x) = t\,e^{iqx} \qquad x > 0\,. \tag{4}$$

In the region $x < 0$ we write

$$\psi_I(x) = e^{ikx} + r\,e^{-ikx} \tag{5}$$

where we have set the coefficient of the incident wave to be 1. There is no loss of generality in this since we will see that ratios of current densities are measured. (Note again that e^{ikx} is traveling to the right and is thus incident on the potential discontinuity) and r and t are the coefficients(amplitudes) of the reflected and transmitted waves respectively. The unknown quantities r and t are determined by using the continuity of ψ and $d\psi/dx$ (denoted by ψ') at $x = 0$. Matching boundary conditions we have

$$\psi_I(x=0): \qquad 1 + r = t \qquad : \psi_{II}(x=0) \tag{6}$$

$$\psi_I'(x=0): \qquad ik(1-r) = iqt \qquad : \psi_{II}'(x=0) \tag{7}$$

which can be solved to obtain

$$r = \frac{k-q}{k+q} \tag{8}$$

$$t = \frac{2k}{k+q} \;. \tag{9}$$

[1] This 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.

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

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

Thus given a wave function $\psi(x) = A\, e^{ikx}$ the current density is $\frac{\hbar k}{m} |A|^2$ which is the velocity of the particle multiplied by the probability density, $|A|^2$. So in region I we have an incident (right-moving) current

$$j_{inc} = \frac{\hbar k}{m}$$

given our choice of the coefficient of 1 and a reflected current (that is left moving) whose magnitude is

$$|j|_{ref} = \frac{\hbar k}{m} |r|^2 .$$

In region II we have a transmitted current

$$j_{trans} = \frac{\hbar q}{m} |t|^2 .$$

The refection and transmission coefficients are defined to be the ratio of the reflected current density to the incident current density and transmitted current density to the incident current density respectively:

$$R \equiv \frac{|j_{ref}|}{j_{inc}} \quad \text{and} \quad T \equiv \frac{j_{tran}}{j_{inc}} \tag{10}$$

Therefore we obtain after some algebraic manipulations

$$R = \frac{(k-q)^2}{(k+q)^2} \quad \text{and} \quad T = \frac{4kq}{(k+q)^2} \quad . \tag{11}$$

You can check that

$$j_{inc} = j_{ref} + j_{tran} \tag{12}$$

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' 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. So as long as we accept the idea that a quantum mechanical particle acts as a wave its behavior becomes more comprehensible.

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

$$\begin{aligned} \psi(x) \;&=\; e^{ikx} \,+\, r\,e^{-ikx} \quad \text{for} \;\; x \,<\, 0 \\ &=\; A\,e^{-\kappa x} \quad \text{where} \;\; \kappa \,=\, \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad \text{for} \;\; x \,>\, 0. \end{aligned} \tag{13}$$

The exponentially increasing solution has been discarded because it is unphysical (the wave function diverges as $x \to \infty$.) Continuity of the wave function and its derivative yield

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

This yields

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

Note that the reflection amplitude r is complex. Since k and κ are real $|\,r\,|^2 = 1$. Make sure you can convince yourself of this and fast. Since $|r| = 1$, r itself can be written in the form $e^{i\phi}$. In the homework problem set you will determine ϕ as a function of k and κ, i.e., as a function of the energy. The reflection coefficient R is just $|r|^2 \;=\; 1$. 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. You can check this is true even though the constant A itself is complex.