Problem 2.34

Consider the "step" potential:[53]

$$V(x) = \begin{cases} 0, & x \le 0, \\ V_0, & x > 0. \end{cases}$$

(a) Calculate the reflection coefficient, for the case $E < V_0$, and comment on the answer.

(b) Calculate the reflection coefficient for the case $E > V_0$.

(c) For a potential (such as this one) that does not go back to zero to the right of the barrier, the transmission coefficient is *not* simply $|F|^2/|A|^2$ (with A the incident amplitude and F the transmitted amplitude), because the transmitted wave travels at a different *speed*. Show that

$$T = \sqrt{\frac{E - V_0}{E}} \frac{|F|^2}{|A|^2}, \tag{2.175}$$

for $E > V_0$. *Hint:* You can figure it out using Equation 2.99, or—more elegantly, but less informatively—from the probability current (Problem 2.18). What is T, for $E < V_0$?

(d) For $E > V_0$, calculate the transmission coefficient for the step potential, and check that $T + R = 1$.

Solution

The governing equation for the wave function $\Psi(x,t)$ is the Schrödinger equation.

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x,t)\Psi(x,t), \quad -\infty < x < \infty,\ t > 0$$

For this step potential,

$$V(x,t) = V(x) = \begin{cases} 0 & \text{if } x \le 0 \\ -V_0 & \text{if } x > 0 \end{cases},$$

which means the PDE becomes

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi(x,t).$$

Since information about the eigenstates and their corresponding energies is desired, the method of separation of variables is opted for. This method works because Schrödinger's equation and its associated boundary conditions (Ψ and its derivatives tend to zero as $x \to \pm\infty$) are linear and homogeneous. Assume a product solution of the form $\Psi(x,t) = \psi(x)\phi(t)$ and plug it into the PDE.

$$i\hbar \frac{\partial}{\partial t}[\psi(x)\phi(t)] = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}[\psi(x)\phi(t)] + V(x)[\psi(x)\phi(t)]$$

Evaluate the derivatives.

$$i\hbar \psi(x)\phi'(t) = -\frac{\hbar^2}{2m}\psi''(x)\phi(t) + V(x)\psi(x)\phi(t)$$

[53] For interesting commentary see C. O. Dib and O. Orellana, *Eur. J. Phys.* **38**, 045403 (2017).

Divide both sides by $\psi(x)\phi(t)$ in order to separate variables.

$$i\hbar\frac{\phi'(t)}{\phi(t)} = -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + V(x)$$

The only way a function of t can be equal to a function of x is if both are equal to a constant E.

$$i\hbar\frac{\phi'(t)}{\phi(t)} = -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + V(x) = E$$

As a result of using the method of separation of variables, the Schrödinger equation has reduced to two ODEs, one in x and one in t.

$$\left.\begin{aligned} i\hbar\frac{\phi'(t)}{\phi(t)} &= E \\ -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + V(x) &= E \end{aligned}\right\}$$

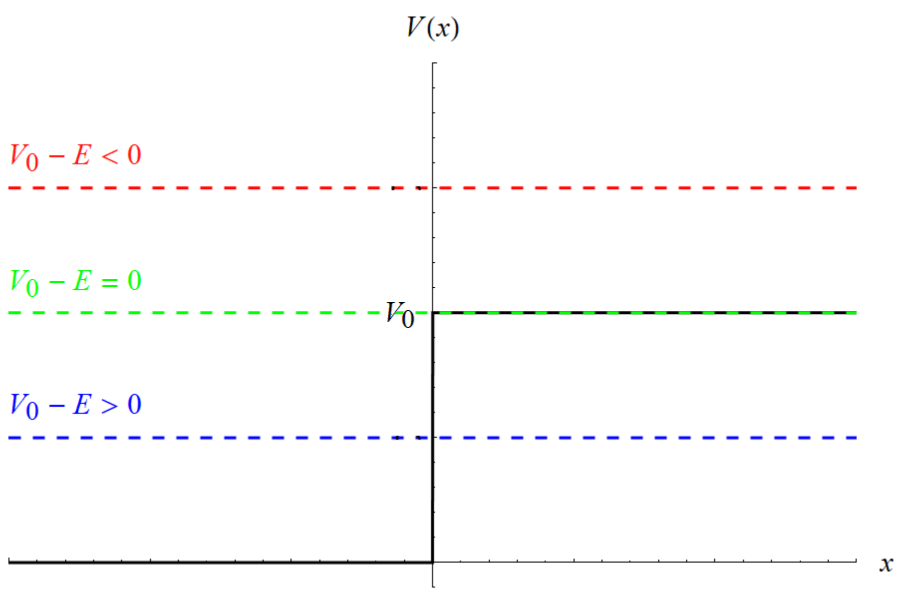
Values of E for which the boundary conditions are satisfied are called the eigenvalues (or eigenenergies in this context), and the nontrivial solutions associated with them are called the eigenfunctions (or eigenstates in this context). The ODE in x is known as the time-independent Schrödinger equation (TISE) and can be written as

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

Split up the ODE over the intervals that $V(x)$ is defined on.

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(-E)\psi, \quad x \leq 0 \qquad\qquad \frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(-V_0 - E)\psi, \quad x > 0$$

The solution for ψ on the interval $x > 0$ depends on whether $V_0 - E > 0$, $V_0 - E = 0$, or $V_0 - E < 0$. Each of these cases will be examined in turn.



Note that scattering states correspond to $E > 0$. In each case, the aim is to determine the reflection and transmission coefficients.

By definition, the reflection coefficient is the ratio of the reflected probability current to the incident probability current. Also, the transmission coefficient is defined to be the ratio of the transmitted probability current to the incident probability current.

$$R = \left|\frac{\text{reflected probability current}}{\text{incident probability current}}\right| \qquad T = \left|\frac{\text{transmitted probability current}}{\text{incident probability current}}\right|$$

The probability current is [noting that $\phi(t) = e^{-iEt/\hbar}$]

$$\begin{aligned} J(x,t) &= \frac{i\hbar}{2m}\left(\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right) \\ &= \frac{i\hbar}{2m}\left\{[\psi(x)e^{-iEt/\hbar}]\frac{\partial}{\partial x}[\psi^*(x)e^{iEt/\hbar}] - [\psi^*(x)e^{iEt/\hbar}]\frac{\partial}{\partial x}[\psi(x)e^{-iEt/\hbar}]\right\} \\ &= \frac{i\hbar}{2m}\left\{[\psi(x)e^{-iEt/\hbar}]\frac{d\psi^*}{dx}e^{iEt/\hbar} - [\psi^*(x)e^{iEt/\hbar}]\frac{d\psi}{dx}e^{-iEt/\hbar}\right\} \\ &= \frac{i\hbar}{2m}\left(\psi\frac{d\psi^*}{dx} - \psi^*\frac{d\psi}{dx}\right). \end{aligned}$$

Case I: $V_0 - E > 0$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi, \quad x \le 0 \qquad\qquad \frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V_0 - E)\psi, \quad x > 0$$

In this case, the general solution on $x > 0$ can be written in terms of exponential functions.

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{if } x \le 0 \\ Fe^{\ell x} + Ge^{-\ell x} & \text{if } x > 0 \end{cases}$$

Here

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

In order to satisfy the boundary condition as $x \to \infty$, set $F = 0$.

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{if } x \le 0 \\ Ge^{-\ell x} & \text{if } x > 0 \end{cases}$$

As a result, the reflection and transmission coefficients are

$$\begin{aligned} R &= \left|\frac{\frac{i\hbar}{2m}\left[(Be^{-ikx})\frac{d}{dx}(B^*e^{ikx}) - (B^*e^{ikx})\frac{d}{dx}(Be^{-ikx})\right]}{\frac{i\hbar}{2m}\left[(Ae^{ikx})\frac{d}{dx}(A^*e^{-ikx}) - (A^*e^{-ikx})\frac{d}{dx}(Ae^{ikx})\right]}\right| \\ &= \left|\frac{(Be^{-ikx})(ikB^*e^{ikx}) - (B^*e^{ikx})(-ikBe^{-ikx})}{(Ae^{ikx})(-ikA^*e^{-ikx}) - (A^*e^{-ikx})(ikAe^{ikx})}\right| \\ &= \left|\frac{2ikBB^*}{-2ikAA^*}\right| \\ &= \frac{|B|^2}{|A|^2} \end{aligned}$$

$$\begin{aligned} T &= \left|\frac{\frac{i\hbar}{2m}\left[(Ge^{-\ell x})\frac{d}{dx}(G^*e^{-\ell x}) - (G^*e^{-\ell x})\frac{d}{dx}(Ge^{-\ell x})\right]}{\frac{i\hbar}{2m}\left[(Ae^{ikx})\frac{d}{dx}(A^*e^{-ikx}) - (A^*e^{-ikx})\frac{d}{dx}(Ae^{ikx})\right]}\right| \\ &= \left|\frac{(Ge^{-\ell x})(-\ell G^*e^{-\ell x}) - (G^*e^{-\ell x})(-\ell Ge^{-\ell x})}{(Ae^{ikx})(-ikA^*e^{-ikx}) - (A^*e^{-ikx})(ikAe^{ikx})}\right| \\ &= \left|\frac{-\ell e^{-2\ell x}GG^* + \ell e^{-2\ell x}GG^*}{-2ikAA^*}\right| \\ &= 0. \end{aligned}$$

To determine one of the constants, require the wave function [and consequently $\psi(x)$] to be continuous at $x = 0$.

$$\lim_{x\to 0^-} \psi(x) = \lim_{x\to 0^+} \psi(x) : \quad A + B = G$$

Integrate both sides of the TISE with respect to x from $-\epsilon$ to ϵ to determine one more.

$$\begin{aligned}\int_{-\epsilon}^{\epsilon} \frac{d^2\psi}{dx^2}\,dx &= \int_{-\epsilon}^{\epsilon} \frac{2m}{\hbar^2}[V(x)-E]\psi(x)\,dx \\ \left.\frac{d\psi}{dx}\right|_{-\epsilon}^{\epsilon} &= \int_{-\epsilon}^{0} \frac{2m}{\hbar^2}(-E)\psi(x)\,dx + \int_{0}^{\epsilon} \frac{2m}{\hbar^2}(V_0-E)\psi(x)\,dx \\ &= -\frac{2mE}{\hbar^2}\psi(0)\int_{-\epsilon}^{0} dx + \frac{2m}{\hbar^2}(V_0-E)\psi(0)\int_0^{\epsilon} dx \\ &= -\frac{2mE}{\hbar^2}\psi(0)\epsilon + \frac{2m}{\hbar^2}(V_0-E)\psi(0)\epsilon\end{aligned}$$

Take the limit as $\epsilon \to 0$.

$$\left.\frac{d\psi}{dx}\right|_{0^-}^{0^+} = 0$$

It turns out that $\partial\Psi/\partial x$ is continuous at $x = 0$ as well.

$$\lim_{x\to 0^-} \frac{d\psi}{dx} = \lim_{x\to 0^+} \frac{d\psi}{dx} : \quad ik(A-B) = -\ell G$$

Substitute the formula for G and solve for B.

$$ik(A-B) = -\ell(A+B)$$

$$B = \frac{-\ell - ik}{\ell - ik}A$$

The reflection coefficient can now be determined.

$$R = \left(\frac{B}{A}\right)\left(\frac{B}{A}\right)^* = \left(\frac{-\ell-ik}{\ell-ik}\right)\left(\frac{-\ell+ik}{\ell+ik}\right) = \frac{\ell^2+k^2}{\ell^2+k^2} = 1$$

Therefore, $R + T = 1$.

Case II: $V_0 - E = 0$

$$\frac{d^2\psi}{dx^2} = -\frac{2mV_0}{\hbar^2}\psi, \quad x \le 0 \qquad\qquad \frac{d^2\psi}{dx^2} = 0, \quad x > 0$$

In this case, the general solution on $x > 0$ is a straight line.

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{if } x \le 0 \\ Fx + G & \text{if } x > 0 \end{cases}$$

Here

$$k = \frac{\sqrt{2mV_0}}{\hbar}.$$

In order to satisfy the boundary condition as $x \to \infty$, set $F = 0$ and $G = 0$.

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{if } x \leq 0 \\ 0 & \text{if } x > 0 \end{cases}$$

Use the continuity of the wave function and its first spatial derivative at $x = 0$ to determine two of the constants.

$$\lim_{x \to 0^-} \psi(x) = \lim_{x \to 0^+} \psi(x) : \quad A + B = 0$$

$$\lim_{x \to 0^-} \frac{d\psi}{dx} = \lim_{x \to 0^+} \frac{d\psi}{dx} : \quad ik(A - B) = 0$$

These equations imply that $A = 0$ and $B = 0$, resulting in the trivial solution: $\psi(x) = 0$. Therefore, $E = V_0$ is not an eigenvalue.

Case III: $V_0 - E < 0$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi, \quad x \leq 0 \qquad\qquad \frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E - V_0)\psi, \quad x > 0$$

In this case, the general solution on $x > 0$ can be written in terms of complex exponential functions.

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{if } x \leq 0 \\ Fe^{ilx} + Ge^{-ilx} & \text{if } x > 0 \end{cases}$$

Here

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

Solving the ODE in t yields $\phi(t) = e^{-iEt/\hbar}$, which means the product solution is a linear combination of waves travelling to the left and to the right.

$$\psi(x)\phi(t) = \begin{cases} Ae^{i(kx - Et/\hbar)} + Be^{-i(kx + Et/\hbar)} & \text{if } x \leq 0 \\ Fe^{i(lx - Et/\hbar)} + Ge^{-i(lx + Et/\hbar)} & \text{if } x > 0 \end{cases}$$

Assuming a plane wave is only incident from the left, set $G = 0$.

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{if } x \leq 0 \\ Fe^{ilx} & \text{if } x > 0 \end{cases}$$

As a result, the reflection and transmission coefficients are

$$\begin{aligned} R &= \left| \frac{\frac{i\hbar}{2m}\left[(Be^{-ikx})\frac{d}{dx}(B^*e^{ikx}) - (B^*e^{ikx})\frac{d}{dx}(Be^{-ikx})\right]}{\frac{i\hbar}{2m}\left[(Ae^{ikx})\frac{d}{dx}(A^*e^{-ikx}) - (A^*e^{-ikx})\frac{d}{dx}(Ae^{ikx})\right]} \right| \\ &= \left| \frac{(Be^{-ikx})(ikB^*e^{ikx}) - (B^*e^{ikx})(-ikBe^{-ikx})}{(Ae^{ikx})(-ikA^*e^{-ikx}) - (A^*e^{-ikx})(ikAe^{ikx})} \right| \\ &= \left| \frac{2ikBB^*}{-2ikAA^*} \right| \\ &= \frac{|B|^2}{|A|^2} \end{aligned}$$

$$\begin{aligned} T &= \left| \frac{\frac{i\hbar}{2m}\left[(Fe^{ilx})\frac{d}{dx}(F^*e^{-ilx}) - (F^*e^{-ilx})\frac{d}{dx}(Fe^{ilx})\right]}{\frac{i\hbar}{2m}\left[(Ae^{ikx})\frac{d}{dx}(A^*e^{-ikx}) - (A^*e^{-ikx})\frac{d}{dx}(Ae^{ikx})\right]} \right| \\ &= \left| \frac{(Fe^{ilx})(-i\ell F^*e^{-ilx}) - (F^*e^{-ilx})(i\ell Fe^{i\ell x})}{(Ae^{ikx})(-ikA^*e^{-ikx}) - (A^*e^{-ikx})(ikAe^{ikx})} \right| \\ &= \left| \frac{-2ilFF^*}{-2ikAA^*} \right| \\ &= \frac{l}{k}\frac{|F|^2}{|A|^2} = \sqrt{\frac{E - V_0}{E}}\frac{|F|^2}{|A|^2}. \end{aligned}$$

To determine one of the constants, require the wave function [and consequently $\psi(x)$] to be continuous at $x = 0$.

$$\lim_{x\to 0^-}\psi(x) = \lim_{x\to 0^+}\psi(x): \quad A + B = F$$

Integrate both sides of the TISE with respect to x from $-\epsilon$ to ϵ to determine one more.

$$\begin{aligned}
\int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}\,dx &= \int_{-\epsilon}^{\epsilon}\frac{2m}{\hbar^2}[V(x)-E]\psi(x)\,dx \\
\left.\frac{d\psi}{dx}\right|_{-\epsilon}^{\epsilon} &= \int_{-\epsilon}^{0}\frac{2m}{\hbar^2}(-E)\psi(x)\,dx + \int_{0}^{\epsilon}\frac{2m}{\hbar^2}(V_0 - E)\psi(x)\,dx \\
&= -\frac{2mE}{\hbar^2}\psi(0)\int_{-\epsilon}^{0}dx + \frac{2m}{\hbar^2}(V_0-E)\psi(0)\int_0^{\epsilon}dx \\
&= -\frac{2mE}{\hbar^2}\psi(0)\epsilon + \frac{2m}{\hbar^2}(V_0-E)\psi(0)\epsilon
\end{aligned}$$

Take the limit as $\epsilon \to 0$.

$$\left.\frac{d\psi}{dx}\right|_{0^-}^{0^+} = 0$$

It turns out that $\partial\Psi/\partial x$ is continuous at $x = 0$ as well.

$$\lim_{x\to 0^-}\frac{d\psi}{dx} = \lim_{x\to 0^+}\frac{d\psi}{dx}: \quad ik(A-B) = ilF$$

To summarize, there are two equations to work with.

$$\begin{cases} A + B = F \\ A - B = \dfrac{l}{k}F \end{cases}$$

Subtract the respective sides to get B.

$$2B = F\left(1 - \frac{l}{k}\right)$$

Solve for B.

$$B = \frac{k-l}{2k}F$$

Add the respective sides to get A.

$$2A = F\left(1 + \frac{l}{k}\right)$$

Solve for F.

$$F = \frac{2k}{k+l}A$$

The transmission coefficient is then

$$\begin{aligned} T = \sqrt{\frac{E-V_0}{E}}\frac{|F|^2}{|A|^2} = \sqrt{\frac{E-V_0}{E}}\left(\frac{F}{A}\right)\left(\frac{F}{A}\right)^* &= \sqrt{\frac{E-V_0}{E}}\left(\frac{2k}{k+l}\right)\left(\frac{2k}{k+l}\right)^* \\ &= \sqrt{\frac{E-V_0}{E}}\left(\frac{2k}{k+l}\right)\left(\frac{2k}{k+l}\right) \\ &= 4\sqrt{\frac{E-V_0}{E}}\left(\frac{1}{1+\frac{l}{k}}\right)\left(\frac{1}{1+\frac{l}{k}}\right) \\ &= 4\sqrt{\frac{E-V_0}{E}}\frac{1}{1+\sqrt{\frac{E-V_0}{E}}}\frac{1}{1+\sqrt{\frac{E-V_0}{E}}} \\ &= \frac{4\sqrt{\frac{E-V_0}{E}}}{1+2\sqrt{\frac{E-V_0}{E}}+\frac{E-V_0}{E}}. \end{aligned}$$

Combine the formulas for B and F.

$$B = \frac{k-l}{2k}F = \frac{k-l}{2k}\left(\frac{2k}{k+l}A\right) = \frac{k-l}{k+l}A$$

The reflection coefficient is then

$$\begin{aligned} R = \frac{|B|^2}{|A|^2} = \left(\frac{B}{A}\right)\left(\frac{B}{A}\right)^* &= \left(\frac{k-l}{k+l}\right)\left(\frac{k-l}{k+l}\right)^* \\ &= \left(\frac{k-l}{k+l}\right)\left(\frac{k-l}{k+l}\right) \\ &= \left(\frac{1-\frac{l}{k}}{1+\frac{l}{k}}\right)\left(\frac{1-\frac{l}{k}}{1+\frac{l}{k}}\right) \\ &= \left(\frac{1-\sqrt{\frac{E-V_0}{E}}}{1+\sqrt{\frac{E-V_0}{E}}}\right)\left(\frac{1-\sqrt{\frac{E-V_0}{E}}}{1+\sqrt{\frac{E-V_0}{E}}}\right) \\ &= \frac{1-2\sqrt{\frac{E-V_0}{E}}+\frac{E-V_0}{E}}{1+2\sqrt{\frac{E-V_0}{E}}+\frac{E-V_0}{E}}. \end{aligned}$$

Therefore,

$$R+T = \frac{1-2\sqrt{\frac{E-V_0}{E}}+\frac{E-V_0}{E}}{1+2\sqrt{\frac{E-V_0}{E}}+\frac{E-V_0}{E}} + \frac{4\sqrt{\frac{E-V_0}{E}}}{1+2\sqrt{\frac{E-V_0}{E}}+\frac{E-V_0}{E}} = \frac{1+2\sqrt{\frac{E-V_0}{E}}+\frac{E-V_0}{E}}{1+2\sqrt{\frac{E-V_0}{E}}+\frac{E-V_0}{E}} = 1.$$