Problem 2.32

Derive Equations 2.170 and 2.171. *Hint:* Use Equations 2.168 and 2.169 to solve for C and D in terms of F:

$$C = \left[\sin(la) + i\frac{k}{l}\cos(la)\right]e^{ika}F; \quad D = \left[\cos(la) - i\frac{k}{l}\sin(la)\right]e^{ika}F.$$

Plug these back into Equations 2.166 and 2.167. Obtain the transmission coefficient, and confirm Equation 2.172.

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 a finite square well,

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

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.

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

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.

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

Scattering states have energy $E > 0$; in this case, the general solution is

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

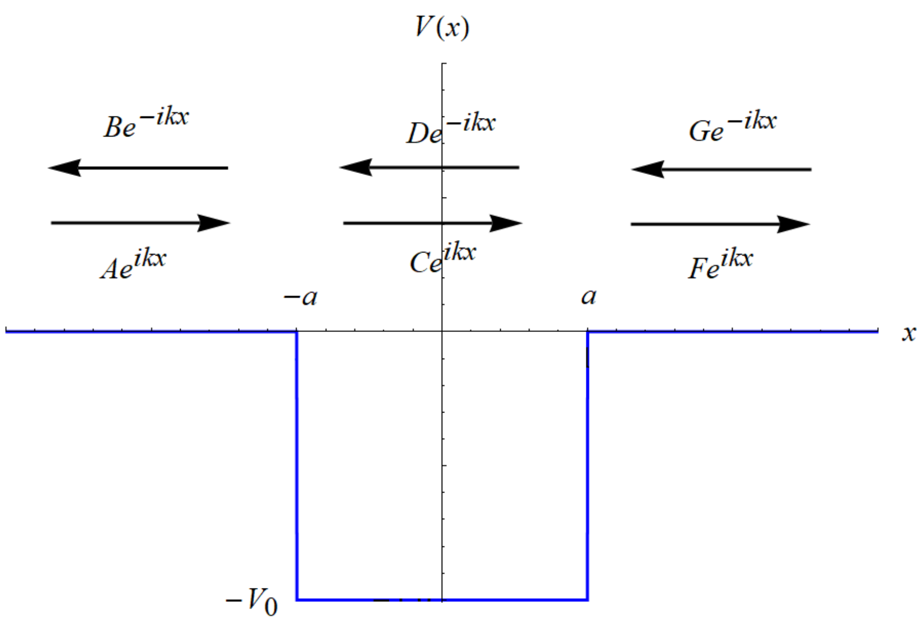
where

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

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.

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

Assuming there's a plane wave incident from the left, $G = 0$, and the reflection and transmission coefficients are $R = |B/A|^2$ and $T = |F/A|^2$, respectively.



In order to simplify the algebra that follows, write the solution inside the well in terms of sine and cosine.

$$\psi(x)=\begin{cases}Ae^{ikx}+Be^{-ikx} & \text{if } x<-a\\ C_0\sin lx+D_0\cos lx & \text{if } -a\leq x\leq a\\ Fe^{ikx}+Ge^{-ikx} & \text{if } x>a\end{cases},$$

Use the fact that the wave function [and consequently $\psi(x)$] is required to be continuous at $x=-a$ and $x=a$ to determine two of the constants.

$$\lim_{x\to-a^-}\psi(x)=\lim_{x\to-a^+}\psi(x):\quad Ae^{-ika}+Be^{ika}=-C_0\sin la+D_0\cos la$$

$$\lim_{x\to+a^-}\psi(x)=\lim_{x\to+a^+}\psi(x):\quad C_0\sin la+D_0\cos la=Fe^{ika}+Ge^{-ika}$$

Integrate both sides of the TISE with respect to x from $-a-\epsilon$ to $-a+\epsilon$, where ϵ is a really small positive number, to determine one more constant.

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

Take the limit as $\epsilon\to0$.

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

$$\lim_{x\to-a^-}\frac{d\psi}{dx}=\lim_{x\to-a^+}\frac{d\psi}{dx}:\quad ik(Ae^{-ika}-Be^{ika})=l(C_0\cos la+D_0\sin la)$$

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

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

Take the limit as $\epsilon\to0$.

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

$$\lim_{x\to a^-}\frac{d\psi}{dx}=\lim_{x\to a^+}\frac{d\psi}{dx}:\quad l(C_0\cos la-D_0\sin la)=ik(Fe^{ika}-Ge^{-ika})$$

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

To summarize, there are four equations involving A, B, C, D, and F. G is set equal to zero.

$$\begin{cases} Ae^{-ika} + Be^{ika} = -C_0 \sin la + D_0 \cos la \\ C_0 \sin la + D_0 \cos la = Fe^{ika} \\ ik(Ae^{-ika} - Be^{ika}) = l(C_0 \cos la + D_0 \sin la) \\ l(C_0 \cos la - D_0 \sin la) = ik(Fe^{ika}) \end{cases}$$

Following the hint, solve the second and fourth equations for C_0 and D_0. Begin by multiplying both sides of the second by $\cos la$ and the fourth by $(\sin la)/l$.

$$\begin{cases} C_0 \sin la \cos la + D_0 \cos^2 la = Fe^{ika} \cos la \\ C_0 \sin la \cos la - D_0 \sin^2 la = \dfrac{ik}{l} Fe^{ika} \sin la \end{cases}$$

Subtract the respective sides to eliminate C_0.

$$D_0(\cos^2 la + \sin^2 la) = Fe^{ika}\left(\cos la - \frac{ik}{l}\sin la\right)$$

$$\boxed{D_0 = Fe^{ika}\left(\cos la - \frac{ik}{l}\sin la\right).}$$

Starting over, multiply both sides of the second by $\sin la$ and the fourth by $(\cos la)/l$.

$$\begin{cases} C_0 \sin^2 la + D_0 \sin la \cos la = Fe^{ika} \sin la \\ C_0 \cos^2 la - D_0 \sin la \cos la = \dfrac{ik}{l} Fe^{ika} \cos la \end{cases}$$

Add the respective sides to eliminate D_0.

$$C_0(\sin^2 la + \cos^2 la) = Fe^{ika}\left(\sin la + \frac{ik}{l}\cos la\right)$$

$$\boxed{C_0 = Fe^{ika}\left(\sin la + \frac{ik}{l}\cos la\right).}$$

Substitute these formulas for C_0 and D_0 into the first equation.

$$\begin{aligned} Ae^{-ika} + Be^{ika} &= -C_0 \sin la + D_0 \cos la \\ &= -Fe^{ika}\left(\sin^2 la + \frac{ik}{l}\sin la \cos la\right) + Fe^{ika}\left(\cos^2 la - \frac{ik}{l}\sin la \cos la\right) \\ &= Fe^{ika}\left(\cos^2 la - \sin^2 la - \frac{2ik}{l}\sin la \cos la\right) \\ &= Fe^{ika}\left(\cos 2la - \frac{ik}{l}\sin 2la\right) \end{aligned}$$

Substitute these formulas for C_0 and D_0 into the third equation.

$$\begin{aligned}\frac{ik}{l}(Ae^{-ika} - Be^{ika}) &= C_0 \cos la + D_0 \sin la \\ &= Fe^{ika}\left(\sin la \cos la + \frac{ik}{l}\cos^2 la\right) + Fe^{ika}\left(\sin la \cos la - \frac{ik}{l}\sin^2 la\right) \\ &= Fe^{ika}\left[2 \sin la \cos la + \frac{ik}{l}(\cos^2 la - \sin^2 la)\right] \\ &= Fe^{ika}\left(\sin 2la + \frac{ik}{l}\cos 2la\right)\end{aligned}$$

Consequently, the first and third equations become

$$\begin{cases} Ae^{-ika} + Be^{ika} = Fe^{ika}\left(\cos 2la - \dfrac{ik}{l}\sin 2la\right) \\ Ae^{-ika} - Be^{ika} = Fe^{ika}\left(\dfrac{l}{ik}\sin 2la + \cos 2la\right) \end{cases}.$$

Subtract the respective sides to get Equation 2.170 in the textbook (page 73).

$$\begin{aligned}2Be^{ika} &= Fe^{ika}\left(\cancel{\cos 2la} - \frac{ik}{l}\sin 2la - \frac{l}{ik}\sin 2la - \cancel{\cos 2la}\right) \\ &= Fe^{ika}\left(\frac{-i^2k^2 - l^2}{ikl}\right)\sin 2la \\ &= Fe^{ika}\left(\frac{k^2 - l^2}{ikl}\right)\sin 2la\end{aligned}$$

Therefore,

$$\boxed{B = i\frac{\sin 2la}{2kl}(l^2 - k^2)F.} \tag{2.170}$$

Add the respective sides to get Equation 2.171 in the textbook (page 73).

$$\begin{aligned}2Ae^{-ika} &= Fe^{ika}\left(\cos 2la - \frac{ik}{l}\sin 2la + \frac{l}{ik}\sin 2la + \cos 2la\right) \\ &= Fe^{ika}\left[2\cos 2la + \left(-\frac{ik}{l} + \frac{l}{ik}\right)\sin 2la\right] \\ &= Fe^{ika}\left[2\cos 2la + \left(\frac{-i^2k^2 + l^2}{ikl}\right)\sin 2la\right] \\ &= 2Fe^{ika}\left[\cos 2la - i\frac{(k^2 + l^2)}{2kl}\sin 2la\right]\end{aligned}$$

Therefore,

$$\boxed{F = \frac{e^{-2ika}A}{\cos 2la - i\frac{(k^2+l^2)}{2kl}\sin 2la}.} \tag{2.171}$$

Use Equation 2.171 to get the transmission coefficient.

$$T = \left|\frac{F}{A}\right|^2 = \left(\frac{F}{A}\right)\left(\frac{F}{A}\right)^* = \left[\frac{e^{-2ika}}{\cos 2la - i\frac{(k^2+l^2)}{2kl}\sin 2la}\right]\left[\frac{e^{2ika}}{\cos 2la + i\frac{(k^2+l^2)}{2kl}\sin 2la}\right]$$
$$= \frac{1}{\cos^2 2la + \frac{(k^2+l^2)^2}{4k^2l^2}\sin^2 2la}$$

Invert both sides and substitute the formulas for k and l.

$$T^{-1} = \cos^2 2la + \frac{(k^2+l^2)^2}{4k^2l^2}\sin^2 2la$$
$$= \cos^2\frac{2a\sqrt{2m(E+V_0)}}{\hbar} + \frac{(2E+V_0)^2}{4E(E+V_0)}\sin^2\frac{2a\sqrt{2m(E+V_0)}}{\hbar}$$
$$= \cos^2\frac{2a\sqrt{2m(E+V_0)}}{\hbar} + \frac{4E^2+4EV_0+V_0^2}{4E(E+V_0)}\sin^2\frac{2a\sqrt{2m(E+V_0)}}{\hbar}$$
$$= \cos^2\frac{2a\sqrt{2m(E+V_0)}}{\hbar} + \cancel{\frac{4E^2+4EV_0}{4E(E+V_0)}}\sin^2\frac{2a\sqrt{2m(E+V_0)}}{\hbar} + \frac{V_0^2}{4E(E+V_0)}\sin^2\frac{2a\sqrt{2m(E+V_0)}}{\hbar}$$

Therefore,

$$\boxed{T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\frac{2a\sqrt{2m(E+V_0)}}{\hbar}.} \tag{2.172}$$

Now combine Equations 2.170 and 2.171.

$$B = i\frac{\sin 2la}{2kl}(l^2-k^2)F = i\frac{\sin 2la}{2kl}(l^2-k^2)\frac{e^{-2ika}A}{\cos 2la - i\frac{(k^2+l^2)}{2kl}\sin 2la}$$

The reflection coefficient is then

$$R = \left|\frac{B}{A}\right|^2 = \left(\frac{B}{A}\right)\left(\frac{B}{A}\right)^*$$
$$= \left[i\frac{\sin 2la}{2kl}(l^2-k^2)\frac{e^{-2ika}}{\cos 2la - i\frac{(k^2+l^2)}{2kl}\sin 2la}\right]\left[-i\frac{\sin 2la}{2kl}(l^2-k^2)\frac{e^{2ika}}{\cos 2la + i\frac{(k^2+l^2)}{2kl}\sin 2la}\right]$$
$$= \frac{\sin^2 2la}{4k^2l^2}(l^2-k^2)^2\frac{1}{\cos^2 2la + \frac{(k^2+l^2)^2}{4k^2l^2}\sin^2 2la}$$
$$= \frac{(l^2-k^2)^2}{4k^2l^2}\frac{\sin^2 2la}{T^{-1}}$$
$$= \frac{V_0^2}{4E(E+V_0)}\frac{\sin^2\frac{2a\sqrt{2m(E+V_0)}}{\hbar}}{1+\frac{V_0^2}{4E(E+V_0)}\sin^2\frac{2a\sqrt{2m(E+V_0)}}{\hbar}} = \frac{1}{\frac{4E(E+V_0)}{V_0^2}\csc^2\frac{2a\sqrt{2m(E+V_0)}}{\hbar}+1}.$$

Therefore,

$$\boxed{R^{-1} = 1 + \frac{4E(E+V_0)}{V_0^2}\csc^2\frac{2a\sqrt{2m(E+V_0)}}{\hbar}.}$$

Note that $R + T = 1$. Below are plots of T versus E and R versus E for the special case that $a = \sqrt{\hbar}$, $m = \hbar$, and $V_0 = 10$.