S2016

Problem 6: Electron in a Finite Square Well (10 pts)

Section 2.6 Griffiths

Consider an electron of energy E incident from x=$-\infty$ on a symmetric one-dimensional square well of depth V_0 and width L.

$$V(x) = \begin{cases} 0, & \text{x < -L/2} \\ -V_0, & \text{-L/2 < x < L/2} \\ 0, & \text{x > L/2} \end{cases}$$

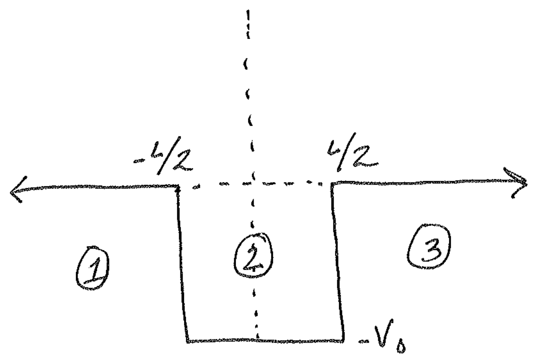
a) Write down the solutions to the time-independent Schrodinger Equation for this situation. There should be five integration constants. (2 points)

b) Apply boundary conditions to find the probability that the electron is transmitted past the finite well. (4 points) (didn't simplify)

c) For what values of E is there a 100% probability for transmission past the well? (2 points)

d) Consider a potential well with V_0 large enough for there to be two bound states. For this well, what is the smallest electron energy (E > 0) for which there is a 100% probability for transmission? Your answer will depend on V_0 and other parameters in the problem. (2 points)

(a)



In general, the time-independent Schrödinger equation is given by

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V\right]\psi = E\psi.$$

In this case, there are three regions to consider, which have been labelled above. We will find the bound states, where $E<0$.

Case 1:

We know $V=0$ for $x<-L/2$, so the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi = E\psi$$

in this region. Letting

$$k = \frac{\sqrt{-2mE}}{\hbar},$$

this becomes

$$\frac{\partial^2\psi}{\partial x^2} = k^2\psi.$$

The general solution to this equation, noting that we can write it as an ordinary differential equation, is

$$\psi(x) = Ae^{-kx} + Be^{kx}, \quad (x<-L/2)$$

where A and B are constants.

(a), cont'd...

Case (2):

We know $V = -V_0$ for $-L/2 < x < L/2$, so the Schrödinger equation is

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V_0\right]\psi = E\psi$$

or

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - (V_0+E)\psi = 0.$$

Letting

$$l = \sqrt{\frac{2m(V_0+E)}{\hbar^2}},$$

this becomes

$$\frac{d^2\psi}{dx^2} = -l^2\psi.$$

The general solution is thus

$$\psi(x) = C\sin(lx) + D\cos(lx), \quad (-L/2 < x < L/2)$$

where C and D are constants.

(a), cont'd...

Case 3:

Again, the Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi,$$

so general solutions in the region $x > L/2$ are

$$\psi(x) = Fe^{-kx} + Ge^{kx}, \quad (x > L/2)$$

where F and G are constants. So, overall we have

$$\psi(x) = \begin{cases} Ae^{-kx} + Be^{kx}, & x < -L/2 \\ C\sin(lx) + D\cos(lx), & -L/2 < x < L/2 \\ Fe^{-kx} + Ge^{kx}, & x > L/2 \end{cases}.$$

Using the properties of the wavefunction, we can simplify this set of expressions. We know the wavefunction must be finite for all x. In region 1, as $x \to -\infty$, the first term grows without bound, so we must have $A = 0$. Similarly, in region 3, as $x \to \infty$, the second term grows without bound and so $G = 0$. Since this potential is an even function, we know the solutions are either even or odd. So, without loss of generality, we let $C = 0$ and assume the solution in region 2 is even. Thus, the solutions to the Schrödinger equation for this potential are

$$\boxed{\psi(x) = \begin{cases} Be^{kx}, & x < -L/2 \\ D\cos(lx), & -L/2 < x < L/2 \\ Fe^{-kx}, & x > L/2 \end{cases}}$$ (for n odd)

where B, D, F, k, and l are constants and

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

(b)

Now we want to consider the scattering states, where $E>0$. In general, we know

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V\right]\psi = E\psi.$$

In region 1, we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi.$$

Letting

$$k = \frac{\sqrt{2mE}}{\hbar},$$

we have

$$\frac{d^2\psi}{dx^2} = -k^2\psi.$$

We know solutions in this region must be exponential in nature, and given the differential equation above, we must have

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \qquad (x < -L/2)$$

where A and B are constants.

The solution in region 2 is unchanged and so

$$\psi(x) = C\sin(lx) + D\cos(lx), \qquad (-L/2 < x < L/2)$$

where C and D are constants, and

$$l = \frac{\sqrt{2m(V_0+E)}}{\hbar}.$$

(b), cont'd...

In region 3, we have

$$\psi(x) = Fe^{ikx} + Ge^{-ikx} \quad , \quad (x > L/2)$$

where F and G are constants. We can say $G = 0$ since we are assuming the only incoming wave is from the left. Then

$$\psi(x) = Fe^{ikx} \quad , \quad (x > L/2).$$

So our wavefunction is

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -L/2 \\ C\sin(lx) + D\cos(lx) \; ; & -L/2 < x < L/2 \\ Fe^{ikx} \; , & x > L/2 \end{cases}$$

where A is the incident wave amplitude, B is the reflected wave amplitude, and F is the transmitted amplitude. We want to determine the transmission coefficient,

$$T = \frac{|F|^2}{|A|^2},$$

by applying our boundary conditions, which state that ψ must be continuous at $x = -L/2$ and $x = L/2$, and similarly for $\frac{d\psi}{dx}$.
So we must have

$$Ae^{ikx} + Be^{-ikx} = C\sin(lx) + D\cos(lx)$$

for $x = -L/2$, or

$$Ae^{-\frac{ikL}{2}} + Be^{\frac{ikL}{2}} = C\sin\left(-\frac{lL}{2}\right) + D\cos\left(-\frac{lL}{2}\right)$$

$$Ae^{-\frac{ikL}{2}} + Be^{\frac{ikL}{2}} = -C\sin\left(\frac{lL}{2}\right) + D\cos\left(\frac{lL}{2}\right). \quad (i)$$

(b), cont'd...

For $d\Psi/dx$ at the first boundary, we have

$$ikAe^{ikx} - ikbe^{-ikx} = lC\cos(lx) - lD\sin(lx)$$

for $x = -L/2$, or

$$ikAe^{-\frac{ikL}{2}} - ikBe^{\frac{ikL}{2}} = lC\cos\left(-\frac{lL}{2}\right) - lD\sin\left(-\frac{lL}{2}\right)$$

$$ikAe^{-\frac{ikL}{2}} - ikBe^{\frac{ikL}{2}} = lC\cos\left(\frac{lL}{2}\right) + lD\sin\left(\frac{lL}{2}\right). \quad \text{(ii)}$$

At our second boundary $(x = L/2)$, we have

$$Fe^{ikx} = C\sin(lx) + D\cos(lx)$$

$$Fe^{\frac{ikL}{2}} = C\sin\left(\frac{lL}{2}\right) + D\cos\left(\frac{lL}{2}\right) \quad \text{(iii)}$$

and

$$ikFe^{ikx} = lC\cos(lx) - lD\sin(lx)$$

$$ikFe^{\frac{ikL}{2}} = lC\cos\left(\frac{lL}{2}\right) - lD\sin\left(\frac{lL}{2}\right) \quad \text{(iv)}.$$

Rearranging (iii) for D, we get

$$D = \frac{Fe^{\frac{ikL}{2}} - C\sin\left(\frac{lL}{2}\right)}{\cos\left(\frac{lL}{2}\right)}.$$

Plugging this into (iv), we have

$$ikFe^{\frac{ikL}{2}} = lC\cos\left(\frac{lL}{2}\right) - l\sin\left(\frac{lL}{2}\right)\left[\frac{Fe^{\frac{ikL}{2}} - C\sin\left(\frac{lL}{2}\right)}{\cos\left(\frac{lL}{2}\right)}\right]$$

$$ikFe^{\frac{ikL}{2}}\cos\left(\frac{lL}{2}\right) = lC\cos^2\left(\frac{lL}{2}\right) - lFe^{\frac{ikL}{2}}\sin\left(\frac{lL}{2}\right) + lC\sin^2\left(\frac{lL}{2}\right)$$

(b), cont'd...

$$ikFe^{\frac{ikL}{2}}\cos\left(\frac{\ell L}{2}\right) = \ell C - \ell Fe^{\frac{ikL}{2}}\sin\left(\frac{\ell L}{2}\right)$$

$$Fe^{\frac{ikL}{2}}\left(ik\cos\left(\frac{\ell L}{2}\right) + \ell\sin\left(\frac{\ell L}{2}\right)\right) = \ell C$$

and so

$$C = Fe^{\frac{ikL}{2}}\left(\frac{ik}{\ell}\cos\left(\frac{\ell L}{2}\right) + \sin\left(\frac{\ell L}{2}\right)\right).$$

Rearranging ⓘ for B, we have

$$Be^{\frac{ikL}{2}} = D\cos\left(\frac{\ell L}{2}\right) - Ae^{-\frac{ikL}{2}} - C\sin\left(\frac{\ell L}{2}\right)$$

$$B = De^{-\frac{ikL}{2}}\cos\left(\frac{\ell L}{2}\right) - Ae^{-ikL} - Ce^{-\frac{ikL}{2}}\sin\left(\frac{\ell L}{2}\right).$$

Plugging this into ⓘⓘ, we have

$$ikAe^{-\frac{ikL}{2}} - ike^{\frac{ikL}{2}}\left[De^{-\frac{ikL}{2}}\cos\left(\frac{\ell L}{2}\right) - Ae^{-ikL} - Ce^{-\frac{ikL}{2}}\sin\left(\frac{\ell L}{2}\right)\right]$$
$$= \ell C\cos\left(\frac{\ell L}{2}\right) + \ell D\sin\left(\frac{\ell L}{2}\right)$$

$$ikAe^{-\frac{ikL}{2}} - ikD\cos\left(\frac{\ell L}{2}\right) + ikAe^{-\frac{ikL}{2}} + ikC\sin\left(\frac{\ell L}{2}\right) = \ell C\cos\left(\frac{\ell L}{2}\right) + \ell D\sin\left(\frac{\ell L}{2}\right)$$

$$2ikAe^{-\frac{ikL}{2}} - D\left(ik\cos\left(\frac{\ell L}{2}\right) + \ell\sin\left(\frac{\ell L}{2}\right)\right) = C\left(\ell\cos\left(\frac{\ell L}{2}\right) - ik\sin\left(\frac{\ell L}{2}\right)\right)$$

Plugging our expression for D into this, we get

$$2ikAe^{-\frac{ikL}{2}} - \left(\frac{Fe^{\frac{ikL}{2}} - C\sin\left(\frac{\ell L}{2}\right)}{\cos\left(\frac{\ell L}{2}\right)}\right)\left(ik\cos\left(\frac{\ell L}{2}\right) + \ell\sin\left(\frac{\ell L}{2}\right)\right)$$
$$= C\left(\ell\cos\left(\frac{\ell L}{2}\right) - ik\sin\left(\frac{\ell L}{2}\right)\right)$$

$$2ikAe^{-\frac{ikL}{2}} - \frac{1}{\cos\left(\frac{\ell L}{2}\right)}\left[ikFe^{\frac{ikL}{2}}\cos\left(\frac{\ell L}{2}\right) + \ell Fe^{\frac{ikL}{2}}\sin\left(\frac{\ell L}{2}\right) - ikC\sin\left(\frac{\ell L}{2}\right)\cos\left(\frac{\ell L}{2}\right)\right.$$
$$\left. - \ell C\sin^2\left(\frac{\ell L}{2}\right)\right] = \left(\ell\cos\left(\frac{\ell L}{2}\right) - ik\sin\left(\frac{\ell L}{2}\right)\right)C$$

$$2ikAe^{-\frac{ikL}{2}}\cos\left(\frac{\ell L}{2}\right) - [\quad] = \ell C\cos^2\left(\frac{\ell L}{2}\right) - ikC\sin\left(\frac{\ell L}{2}\right)\cos\left(\frac{\ell L}{2}\right)$$

(b), cont'd...

$$2ikAe^{-\frac{ikL}{2}}\cos\left(\frac{lL}{2}\right) - ikFe^{\frac{ikL}{2}}\cos\left(\frac{lL}{2}\right) - lFe^{\frac{ikL}{2}}\sin\left(\frac{lL}{2}\right)$$
$$= C\left[l\left(\cos^2\left(\frac{lL}{2}\right) - \sin^2\left(\frac{lL}{2}\right)\right) - 2ik\sin\left(\frac{lL}{2}\right)\cos\left(\frac{lL}{2}\right)\right]$$
$$= C\left[l\cos(lL) - ik\sin(lL)\right]$$

Plugging in our expression for C, we have

$$2ikAe^{-\frac{ikL}{2}}\cos\left(\frac{lL}{2}\right) - Fe^{\frac{ikL}{2}}\left(ik\cos\left(\frac{lL}{2}\right) + l\sin\left(\frac{lL}{2}\right)\right)$$
$$= \left(Fe^{\frac{ikL}{2}}\left(\frac{ik}{l}\cos\left(\frac{lL}{2}\right) + \sin\left(\frac{lL}{2}\right)\right)\right)\left[l\cos(lL) - ik\sin(lL)\right]$$

Dividing by $Fe^{\frac{ikL}{2}}$, we get

$$2ike^{-ikL}\frac{A}{F}\cos\left(\frac{lL}{2}\right) - \left(ik\cos\left(\frac{lL}{2}\right) + l\sin\left(\frac{lL}{2}\right)\right)$$
$$= \left(\frac{ik}{l}\cos\left(\frac{lL}{2}\right) + \sin\left(\frac{lL}{2}\right)\right)\left(l\cos(lL) - ik\sin(lL)\right)$$

$$2ike^{-ikL}\cos\left(\frac{lL}{2}\right)\frac{A}{F} = \frac{1}{l}\left(ik\cos\left(\frac{lL}{2}\right) + l\sin\left(\frac{lL}{2}\right)\right)\left(l\cos(lL) - ik\sin(lL)\right)$$
$$+ \left(ik\cos\left(\frac{lL}{2}\right) + l\sin\left(\frac{lL}{2}\right)\right)$$
$$= \left(ik\cos\left(\frac{lL}{2}\right) + l\sin\left(\frac{lL}{2}\right)\right)\left(\cos(lL) - \frac{ik}{l}\sin(lL) + 1\right)$$

So

$$\frac{A}{F} = \frac{\left[ik\cos\left(\frac{lL}{2}\right) + l\sin\left(\frac{lL}{2}\right)\right]\left[\cos(lL) - \frac{ik}{l}\sin(lL) + 1\right]}{2ike^{-ikL}\cos\left(\frac{lL}{2}\right)}$$

or

$$\frac{F}{A} = \frac{2ike^{-ikL}\cos\left(\frac{lL}{2}\right)}{\left[ik\cos\left(\frac{lL}{2}\right) + l\sin\left(\frac{lL}{2}\right)\right]\left[\cos(lL) - \frac{ik}{l}\sin(lL) + 1\right]}$$

(b), cont'd...

Now we need

$$T = \frac{|F|^2}{|A|^2}.$$

Taking the complex square, we get

$$T = \frac{|F|^2}{|A|^2} = \left[\frac{2ike^{-ikL}\cos\left(\frac{lL}{2}\right)}{\left(ik\cos\left(\frac{lL}{2}\right)+l\sin\left(\frac{lL}{2}\right)\right)\left(\cos(lL)-\frac{ik}{l}\sin(lL)+1\right)}\right]$$

$$\cdot\left[\frac{2(-i)ke^{+ikL}\cos\left(\frac{lL}{2}\right)}{\left((-i)k\cos\left(\frac{lL}{2}\right)+l\sin\left(\frac{lL}{2}\right)\right)\left(\cos(lL)+\frac{ik}{l}\sin(lL)+1\right)}\right]$$

$$\boxed{T = \frac{4k^2\cos^2\left(\frac{lL}{2}\right)}{\left(k^2\cos^2\left(\frac{lL}{2}\right)+l^2\sin^2\left(\frac{lL}{2}\right)\right)\left(\cos^2(lL)+2\cos(lL)+\frac{k^2}{l^2}\sin^2(lL)+1\right)}}$$

Not really sure how to simplify this, but this is the probability that the electron is transmitted past the well, where again,

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$l = \frac{\sqrt{2m(V_0+E)}}{\hbar}.$$

So the probability only depends on E, V_0, and the width of our well, as expected.

(c)

A 100% probability for transmission past the well corresponds to a transmission coefficient of

$$T = 1.$$

In order to determine what values of E correspond to this probability, I would set the expression for T from part (b) equal to 1 and solve for E. The only way for the numerator and denominator to be equal is if we have

$$\frac{\ell L}{2} = n\pi .$$

Plugging in our expression for ℓ, then rearranging for E, we get

$$\frac{L}{2}\left(\frac{\sqrt{2m(V_0+E)}}{\hbar}\right) = n\pi$$

$$\sqrt{2m(V_0+E)} = \frac{2n\hbar\pi}{L}$$

$$2m(V_0+E) = \frac{4n^2\hbar^2\pi^2}{L^2}$$

$$V_0 + E = \frac{2n^2\hbar^2\pi^2}{mL^2}$$

$$\boxed{E = \frac{2n^2\hbar^2\pi^2}{mL^2} - V_0}$$