Review

Finite square well

Tunneling

Approximate energy solution

Review

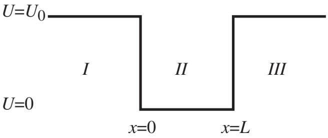
- We have looked at several examples of the time-independent Schrödinger equation:

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

- We have solved the infinite quantum well.
- We have looked at the quantum mechanical harmonic oscillator:
  - The ground state looks like $\psi = A\exp[-ax^2]$.
  - The length scale is $a = \sqrt{km}/2\hbar$, but particles can go farther than the classical limit. However, larger excursions are exponentially killed. . .
  - The state energies go like $E_n = (n + \frac{1}{2}\hbar\omega)$ with $n = 0, 1, 2, \ldots$
  - At zero temperature, motion does *not* cease! Zero temperature means all particles are in their ground state.
- We also talked about the meaning of ψ (probability amplitude) and ψ^2 (probability).

Finite square well (Serway 6.5)

- We've done a particle in a restoring force potential (the harmonic oscillator), and also in an infinite square well. Let's now consider a finite square well!



- Based on our solution to the harmonic oscillator, we expect that a particle should be sort-of confined but that it might extend out past its classical limit.
- Outside the well (regions *I* and *III*), Schrödinger's equation for a particle traveling in a constant finite potential is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U_0\psi = E\psi$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (U_0 - E)\psi$$

$$\frac{d^2\psi}{dx^2} = \alpha^2\psi \quad \text{with} \quad \alpha^2 \equiv \frac{2m(U_0 - E)}{\hbar^2}$$

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Finite square well II

- Again, for outside the finite square well (regions *I* and *III*) we had

$$\frac{d^2\psi}{dx^2} = \alpha^2\psi \qquad \text{with} \qquad \alpha^2 \equiv \frac{2m(U_0 - E)}{\hbar^2}$$

  Now in the case where $E > U_0$ we have a particle which happily travels along with a different net energy and thus a different de Broglie wavelength, and the particle will never be bound inside the finite square well. So let's consider only the cases where $E < U_0$. In this case, α^2 is always a positive number, and two possible solutions for the wave function are $\psi = Ae^{+\alpha x}$ and $\psi = Ae^{-\alpha x}$.

- Consider region *I*. If we were to have $\psi = Ae^{-\alpha x}$ then the wave function ψ would grow exponentially as we went to increasing $-x$ values farther away from the confining potential. This would require exponentially increasing energy! The converse holds for region *III*. The solutions that *do* make sense for regions *I* and *III* are

$$\psi_I(x) = Ae^{+\alpha x} \qquad \text{and} \qquad \psi_{III}(x) = De^{-\alpha x}$$

Finite square well III

- What we have seen is that in region *III* for example we have a wavefunction which is a decaying exponential:

$$\psi_{III}(x) = Ae^{-\alpha x} \qquad \text{with} \qquad \alpha \equiv \frac{\sqrt{2m(U_0 - E)}}{\hbar}$$

  That is, the wavefunction $\psi_{III}(x)$ dies off to $1/e$ of its amplitude in a distance δ of $1/\alpha$, or

$$\delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(U_0 - E)}} \tag{1}$$

- The probability $\propto \psi^2$ will be attenuated by $\exp[-1] = \exp[-1/2]^2 = e^{-\left(\frac{1}{2}\right)^2} = 0.37$ when we have traveled a tunneling distance x_t of $\delta/2$.

From infinite to finite quantum well

- Recall that for quantum well of width L with infinite sides, we found that the energies of allowed states were given by

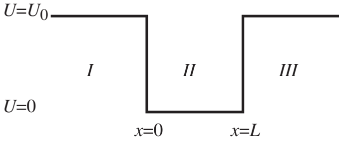
$$E_n = \frac{n^2\pi^2 h^2}{2mL^2} \qquad \text{for} \qquad n = 1, 2, \ldots$$

- We can get a first order approximation of the energies of states in the *finite* quantum well by increasing the width of an infinite box by δ on each side:

$$E_n \simeq \frac{n^2\pi^2 h^2}{2m(L+2\delta)^2} \qquad \text{for} \qquad n = 1, 2, \ldots \tag{2}$$

Finite square well IV

- Let's return to the wave function characteristics. We found $\psi_I = Ae^{+\alpha x}$ and $\psi_{III} = De^{-\alpha x}$, with $\alpha = \sqrt{2m(U_0 - E)}/\hbar$. What about inside the potential, in region *II*?



- Well, here we have a free particle in zero potential which can travel either direction, which we could write as $\psi_{II}(x) = Be^{-ikx} + Ce^{+ikx}$ but since $e^{ikx} = \sin kx + i \cos kx$ we can also write this as

$$\psi_{II}(x) = B \sin(kx) + C \cos(kx) \text{ with } k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{\sqrt{2mE}}{\hbar}. \tag{3}$$

- Now that we have forms for the wave function in each region, we require the wave function to be continuous and un-kinked.

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Boundary conditions in general, and at $x = 0$

- We want the wavefunction to be continuous. We have the wave functions; to get them to be unkinked we need their derivatives:

$$
\begin{aligned}
\frac{d\psi_I}{dx} &= \tfrac{d}{dx} A e^{+\alpha x} &&= A\alpha e^{+\alpha x} \\
\frac{d\psi_{II}}{dx} &= \tfrac{d}{dx}\left(B\sin(kx) + C\cos(kx)\right) &&= Bk\cos(kx) - Ck\sin(kx) \\
\frac{d\psi_{III}}{dx} &= \tfrac{d}{dx} D e^{-\alpha x} &&= -D\alpha e^{-\alpha x}
\end{aligned}
$$

- Now let's consider $x = 0$ which is the boundary between regions I and II. We want to satisfy

$$
\begin{aligned}
A e^{+\alpha\cdot 0} &= B\sin(k\cdot 0) + C\cos(k\cdot 0) &&\Rightarrow\ A = C \\
\text{and } A\alpha e^{+\alpha\cdot 0} &= Bk\cos(k\cdot 0) - Ck\sin(k\cdot 0) &&\Rightarrow\ A\alpha = Bk
\end{aligned}
$$

which gives $A = C = Bk/\alpha$.

Boundary conditions at $x = L$

Now let's look at the right boundary. From continuity of the wavefunctions and $C = Bk/\alpha$ we get

$$B\sin(kL) + C\cos(kL) = B\sin(kL) + B\frac{k}{\alpha}\cos(kL) = De^{-\alpha L} \qquad (4)$$

while from the continuity of the derivative we get

$$Bk\cos(kL) - Ck\sin(kL) = Bk\cos(kL) - B\frac{k^2}{\alpha}\sin(kL) = -D\alpha e^{-\alpha L}. \qquad (5)$$

The ratio of these two expressions is

$$\frac{\sin(kL) + \frac{k}{\alpha}\cos(kL)}{\cos(kL) - \frac{k}{\alpha}\sin(kL)} = -\frac{k}{\alpha}. \qquad (6)$$

While this is nothing that is easily simplified, we can still gain some insight into the solution.

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What have we learned from the boundary conditions?

- We have found that the boundary conditions let us relate $A = C = Bk/\alpha$ and once we know a particular energy solution (and thus $k = \sqrt{2mE}/\hbar$) we can get a relationship to coefficient D from Eq. 4.
- More importantly, we have arrived at the relationship of Eq. 5 of

$$\frac{\sin(kL) + \frac{k}{\alpha}\cos(kL)}{\cos(kL) - \frac{k}{\alpha}\sin(kL)} = -\frac{k}{\alpha}.$$

where $k = \sqrt{2mE}/\hbar$ and $\alpha = \sqrt{2m(U_0 - E)}/\hbar$, or

$$\frac{\sin(\sqrt{2mE}\frac{L}{\hbar}) + \sqrt{\frac{E}{U_0 - E}}\cos(\sqrt{2mE}\frac{L}{\hbar})}{\cos(\sqrt{2mE}\frac{L}{\hbar}) - \sqrt{\frac{E}{U_0 - E}}\sin(\sqrt{2mE}\frac{L}{\hbar})} = -\sqrt{\frac{E}{U_0 - E}}. \quad (7)$$

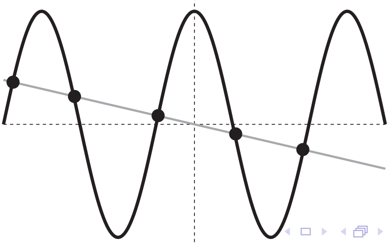
So what can we do with this?

What does this tell us?

Again, by matching boundary conditions we have found the requirement of Eq. 7:

$$\frac{\sin(\sqrt{2mE}\frac{L}{\hbar}) + \sqrt{\frac{E}{U_0-E}}\cos(\sqrt{2mE}\frac{L}{\hbar})}{\cos(\sqrt{2mE}\frac{L}{\hbar}) - \sqrt{\frac{E}{U_0-E}}\sin(\sqrt{2mE}\frac{L}{\hbar})} = -\sqrt{\frac{E}{U_0 - E}}.$$

This is of course not straightforward to solve! However, if we know L, m, and U_0, we can at least plot the left hand side versus E, and we can also plot the right hand side versus E. This allows us to find a discrete set of solutions! Let's say the left hand side was a simple cosine function, and the right hand side was a simple linear slope; we'd then find particular energy solutions graphically as follows:



Finite square well: the picture

OK, so you get the idea. The wavefunction solutions ψ at the discrete energy states look like this (Serway Fig. 6.16):

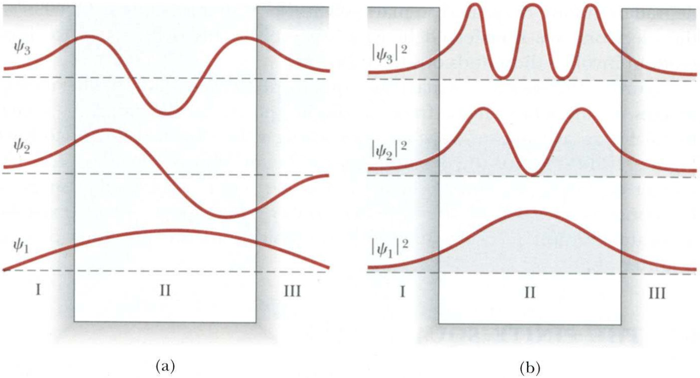
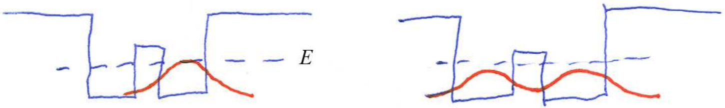


Figure 6.16 (a) Wavefunctions for the lowest three energy states for a particle in a potential well of finite height. (b) Probability densities for the lowest three energy states for a particle in a potential well of finite height.

To dive into this some more, try Serway problem 6.23!

Leaking/sloshing states

- Consider two finite wells with a reduced barrier between them. If we put a classical particle in one well, with less energy than the height of the barrier, it's stuck in that well forever.
- Not so with quantum mechanics! The particle can "leak" out of one well and into the other! Particles can slosh back and forth between these two wells, and end up distributed between them:



- Which well is the particle in? Both! This is a better situation to visualize than Schrödinger's cat being both alive and dead.