Lecture 16

1 Solving the Schrödinger Equation for $\hat{E}$ eigenfunctions: Examples

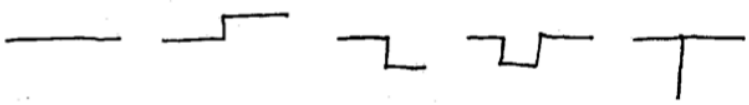
3 forms:

$$i\hbar\partial_t\psi(x,t) = -\frac{\hbar^2}{2m}\partial_x^2\psi(x,t) + V(x)\psi(x,t) \quad (1)$$

$$E\phi_E(x) = -\frac{\hbar^2}{2m}\partial_x^2\phi_E(x) + V(x)\phi_E(x) \quad (2)$$

$$\phi_E''(x) = \frac{2m}{\hbar^2}(V(x) - E)\phi_E(x) \quad (3)$$

Today, here are the various situations we are going to solve the S.E. for:



The key to solving the S.E. in each of these situations is to use a piecewise constant. The strategy is: solve the equation in each constant region, then match separate regions at their boundaries.

Recall: Continuity of $\phi_E(x)$

- If $V(x)$ jumps finitely, then so does $\phi_E''(x)$. Therefore, ϕ' and ϕ are continuous.
- If $V(x)$ jumps to infinity, then so does $\phi_E''(x)$. Therefore, ϕ' jumps finitely, and ϕ_E is continuous.

1.1 Example 1: Free Particle, V(x) = 0

The generation solution of the S.E.:

$$\phi''_E(x) = Ae^{ikx} + Be^{-ikx} \tag{4}$$

where

$$E = \frac{\hbar^2 k^2}{2m} \tag{5}$$

To see the meaning of this, let's add time evolution.

$$\phi''_E(x) = Ae^{ikx-\omega t} + Be^{-ikx+\omega t} \tag{6}$$

where

$$\omega = \frac{E}{\hbar} \tag{7}$$

We see that the first part of the expression describes a phase moving right, and the second part describes a phase moving left. So, the wavefunction ϕ_E is a superposition of right- and left-moving waves.

Note: ϕ_E is not normalizable. Rather, $\langle \phi_E | \phi_{E'} \rangle = \delta(E - E')$. To describe a single particle, we must build normalizable wavepackets. How do they behave?

Example: Consider a minimum uncertainty wavefunction,

$$\psi(x, 0) = \frac{1}{(\pi a^2)^{1/4}} e^{-\frac{x^2}{2a^2}} \tag{8}$$

What is $\psi(x, t)$?

Our strategy is the same as usual: given $\psi(x, 0)$, we can expand it as a superposition of $\hat{E}$ eigenstates, then use the S.E. to evolve each term in the superposition. Let's do it explicitly:

1. Expand in energy eigenstates

$$\hat{E}\left(\frac{1}{2\pi}e^{ikx}\right) = \frac{\hbar^2 k^2}{2m}\left(\frac{1}{2\pi}e^{ikx}\right) \tag{9}$$

$$\psi(x,0) = \int dk \left(\frac{1}{2\pi}e^{ikx}\right)\tilde{\psi}(k) \tag{10}$$

Note: We usually call that $\tilde{\psi}(k)$ term c_n, but in this case it's just the Fourier transform!

$$= \int dk \left(\frac{1}{2\pi}e^{ikx}\right)\left(4\sqrt{\frac{a^2}{\pi}}e^{-\frac{a^2k^2}{2}}\right) \tag{11}$$

You showed this in Problem Set 2.

2. Time evolve the stationary states

$$\psi(x,0) = \int dk \left(\frac{1}{2\pi}e^{i(kx-\omega t)}\right)\left(\frac{a^2}{\pi}\right)^{1/4} e^{-\frac{a^2k^2}{2}} \tag{12}$$

3. In principle, we are done. However, since we know that $\omega(k) = \frac{\hbar k^2}{2m}$, we can actually do the k integral:

$$\begin{aligned}
\psi(x,t) &= \int \frac{dk}{\sqrt{2\pi}} e^{ikx - i\frac{\hbar k^2}{2m}t - \frac{a^2k^2}{2}} \left(\frac{a^2}{\pi}\right)^{1/4} && (13)\\
&= \left(\frac{a^2}{\pi}\right)^{1/4} \int \frac{dk}{\sqrt{2\pi}} e^{ikx} e^{-\frac{k^2}{2}(a^2 + i\frac{\hbar}{2m}t)} && (14)\\
& && (15)
\end{aligned}$$

The $e^{ikx}e^{-\frac{k^2}{2}(a^2+i\frac{\hbar}{2m}t)}$ is just another Gaussian! But we know the Fourier transform of a Gaussian...

$$\psi(x,t) = \left(\frac{a^2}{\pi}\right)^{1/4} \int \frac{dk}{\sqrt{2\pi}} e^{ikx} e^{-\frac{k^2a^2(t)}{2}} \tag{16}$$

where

$$a^2(t) = a^2 + i\frac{\hbar}{m}t \tag{17}$$

From our results about Gaussian integration, we can just plug in $a^2(t)$ to get,

$$\psi(x,t) = \left(\frac{a^2}{\pi(a^2(t))^2}\right) e^{-\frac{x^2}{2a^2(t)}} \tag{18}$$

where

$$a^2(t) = a^2 + i\frac{\hbar}{m}t \tag{19}$$

As a check, at $t = 0$ this reproduces to our original Gaussian.

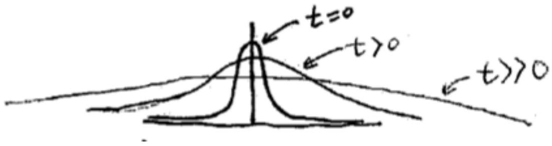
4. To see more precisely what this means, let's look at $\mathbf{P}(x,t)$

$$P(x,t) = |\psi(x,t)|^2 = \frac{\pi^{-1/4}}{a^2 + (\frac{\hbar}{ma})^2 t^2} e^{-\frac{x^2}{(a^2+(\frac{\hbar}{ma})^2 t^2)}} \tag{20}$$

Check:

- $[\frac{\hbar}{ma}]$ is proportional to velocity, check
- When t goes to 0, it reduces to the original Gaussian squared, check

5. Graphically,



so the wavefunction **spreads out** or **disperses!** This is what we saw in the first simulation in class!

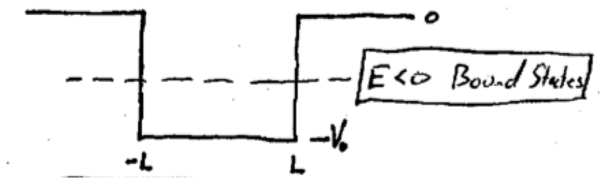
6. Two questions to get you thinking:

   (a) The width in this example is smallest at $t = 0$. Why? How could you build a $\psi(x,0)$ whose width is smallest at some time $t = T$?

   (b) How would you make the wavepacket move? Hint: what is $\psi(x,t)$ if $\psi(x,0) = Ne^{-\frac{x^2}{2a}}e^{ik_0x}$

1.2 Finite Well, cont.

Note: $V(x)$ is symmetric, so the wavefunction must be symmetric or antisymmetric!



$$E\phi_E = \frac{-\hbar^2}{2m}\phi_E''(x) + V(x)\phi_E(x) \tag{21}$$

rearranges to

$$\phi_E''(x) = \frac{2m}{\hbar^2}(V(x) - E)\phi_E(x) \tag{22}$$

Defining $V(x)$ by the above graph, there are two types of regions for the bound states, for which $0 > E > -V_0$:

"Classically allowed":	$\lvert x\rvert < L$	$\phi'' = -k^2\phi$	$k = \sqrt{\frac{2m}{\hbar^2}(E + V_0)}$
"Classically forbidden":	$\lvert x\rvert > L$	$\phi'' = -\alpha^2\phi$	$\alpha = \sqrt{\frac{2m}{\hbar^2}(-E)}$

Note: $k^2 + \alpha^2 = \frac{2mV_0}{\hbar^2}$

General Solution:

$$\phi_E(x) = \begin{cases} Ce^{\alpha x} + \cancel{De^{-\alpha x}} & \text{to the left of the well} \\ A\cos kx + B\sin kx & \text{inside the well} \\ \cancel{Ee^{\alpha x}} + Fe^{-\alpha x} & \text{to the right of the well} \end{cases}$$

For normalizability, $\phi(x \to -\infty) \to 0$ so $D = 0$. Similarly, $\phi(x \to +\infty) \to 0$ so $E = 0$.

We need parity, so the even solution requires $B = 0$ and $C = F$. The odd solution requires $A = 0$, $F = -C$. Therefore:

$$\phi_E^{even}(x) = \begin{cases} Ce^{\alpha x} & \text{to the left of the well} \\ B\sin kx & \text{inside the well} \\ -Ce^{-\alpha x} & \text{to the right of the well} \end{cases}$$

$$\phi_E^{odd}(x) = \begin{cases} Ce^{\alpha x} & \text{to the left of the well} \\ A\cos kx & \text{inside the well} \\ Ce^{-\alpha x} & \text{to the right of the well} \end{cases}$$

We still need to impose continuity conditions at $x = \pm L$! Here, ϕ and ϕ' must be continuous.

$$\phi : A\cos(kL) = Ce^{-\alpha L} \tag{23}$$

$$\phi' : -Ak\sin(kL) = -C\alpha e^{-\alpha L} \tag{24}$$

Combining 23 and 24, we get

$$k\tan kL = \alpha \tag{25}$$

At $x = -L$, we have the same conditions (check this). This equation is rewritten below, along with the definitions of κ and α. Every solution to these three equations specifies an eigenfunction and it's energy.

$$kL\tan kL = \alpha L \tag{26}$$

$$k^2 = \frac{2m}{\hbar^2}(V_0 + E) \tag{27}$$

$$\alpha^2 = \frac{2m}{\hbar^2}(-E) \tag{28}$$

To begin solving these transcendental equations, we simplify life with dimensionless variables. Let $z = kL$ and $\alpha L = y$. Note: $z^2 + y^2 = L^2(\frac{2m}{\hbar^2}V_0) \equiv \mathbb{R}_0^2$. So, continuity conditions:

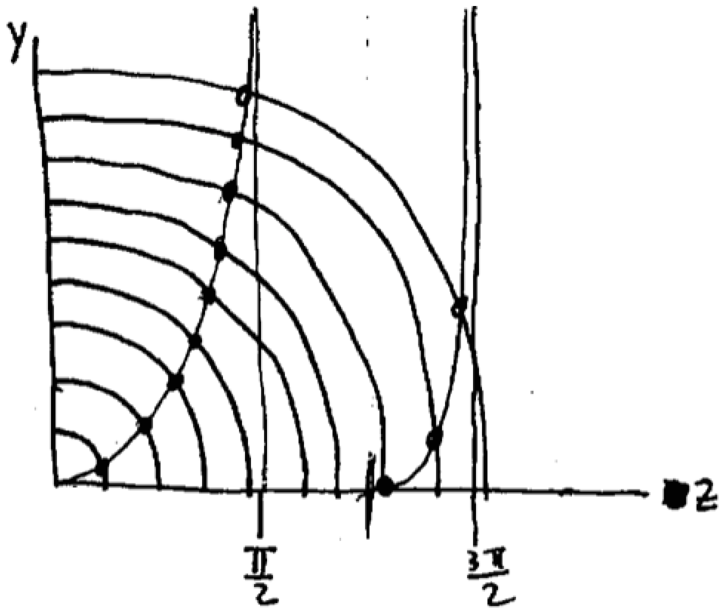
$$\mathbb{R}_0^2 = z^2 + y^2 \tag{29}$$

$$y = z\tan z \tag{30}$$

Solutions with $y, z > 0$ correspond to solutions of $\hat{E}\phi_E(x) = E\phi_E(x)$ which satisfy the boundary conditions at $x = \pm L$. A plot is shown below.

Larger V_0, corresponding to a deeper well, means bigger circles. Note that there is always at least one even solution. Note, too, that there is a new solution (corresponding to the first excited state) at $z = \pi, y = 0$.

Check: Do we get an infinite well in the limit $V_0 \to \infty$? Well, $V_0 \to \infty \Rightarrow \mathbb{R}_0 \to \infty \Rightarrow z = (n + \frac{1}{2})\pi \Rightarrow kL = \frac{2n+1}{2}\pi \Rightarrow k_n = \frac{(2n+1)\pi}{2L}$. The $(2n+1)$ tells us we only have even



numbers, and the width is $2L$. This is correct.

Normalization?

$$1 = \int_{-\infty}^{\infty} dx |\phi_E|^2 = \int_{-\infty}^{-L} dx |C|^2 e^{2\alpha x} + \int_{-L}^{L} dx |A|^2 \cos^2 kL + \int_{L}^{\infty} dx |F|^2 e^{-2\alpha x}$$

Recall ($C = Ae^{\alpha L} \cos kL$) $\Rightarrow$ $\alpha L = kL \tan kL \Rightarrow C = \frac{e^{\alpha L} \cos kL}{\sqrt{L+\frac{1}{\alpha}}} = F$ and $A = \frac{1}{\sqrt{L+\frac{1}{\alpha}}}$

Note: If we take $V_0 \to \infty, L \to 0$ and keep constant area $= 2L \cdot V_0 =$ const, we get $V(x) \to -V_0 \delta(x)$