Last Time: free particle $V(x) = V_0$ general solution

$$\psi = Ae^{ikx} + Be^{-ikx}$$

A, B are complex constants, determined by “boundary conditions”

$$k = \frac{p}{\hbar} \quad \text{(from } e^{ikx}, \text{ eigenfunction of } \hat{p}, \text{ and the real number, } p, \text{ is the eigenvalue)}$$

$$k = \left[ (E - V_0) \frac{2m}{\hbar^2} \right]^{1/2} \quad \text{for } E \geq V_0$$

probability distribution

$$P(x) = \psi^* \psi = |A|^2 + |B|^2 + 2 \text{Re}(A*B) \cos 2kx + 2 \text{Im}(A*B) \sin 2kx$$

only get wiggly stuff when 2 or more different values of k are superimposed. In this special case we had $+k$ and $-k$.

TODAY

1. infinite box
2. $\delta(x)$ well
3. $\delta(x)$ barrier
What do we know about $\psi(x)$ for physically realistic $V(x)$?

$\psi(\pm \infty) =$ ?

$\psi^*(x)\psi(x)$ for all $x$?

$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx$?

Continuity of $\psi$ and $d\psi/dx$?

Computationally convenient potentials have steps and flat regions.

- Infinite step
- Finite step
- Infinitely high but infinitely thin step, “$\delta$-function”

$\psi$ continuous

$\frac{d\psi}{dx}, \frac{d^2\psi}{dx^2}$ not continuous for infinite step, and not for $\delta$-function

$\frac{d\psi}{dx}$ is continuous for finite step

More warm up exercises

1. Infinite box

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

$[C=A+B, D=iA - iB]$

$\psi(0) = 0 \Rightarrow C = 0$

$\psi(L) = 0 \Rightarrow kL = n\pi \quad n = 1, 2, \ldots$ (why not $n = 0$?)
\[
\begin{aligned}
\text{recall} & \quad k^2 = (E - V_0) \frac{2m}{\hbar^2} = \frac{n^2 \pi^2}{L^2} \quad \text{here.} \\
E_n &= n^2 \frac{\hbar^2 \pi^2}{2mL^2} = n^2 \left[ \frac{\hbar^2}{8mL^2} \right] \\
\end{aligned}
\]

Insert kL = n\pi boundary condition.

\[
E_n = n^2 \frac{\hbar^2 \pi^2}{2mL^2} = n^2 \left[ \frac{\hbar^2}{8mL^2} \right]
\]

\[
\begin{align*}
\int_0^L D dx \sin^2(n\pi x) & \quad \Rightarrow \\
\psi_n(x) &= (2/L)^{1/2} \sin(n\pi x)
\end{align*}
\]

\[
\begin{aligned}
1 = |D|^2 \int_0^L dx \sin^2(n\pi x) & \quad \Rightarrow \\
D &= (2/L)^{1/2} \sqrt{\frac{\pi}{\int_0^L \sin^2(n\pi x) dx}} = \frac{L}{2} \\
\end{aligned}
\]

 carts of $\psi_n(x)$: what happens to $\{\psi_n\}$ and $\{E_n\}$ if we move well:

- left or right in $x$?
- up or down in $E$?

Infinite well was easy: 2 boundary conditions plus normalization requirement.

Generalize to stepwise constant potentials: in each V(x)=constant region, need to know 2 complex coefficients and, if the particle is confined within a finite range of $x$, there is quantization of energy.

* boundary and joining conditions
* normalization
* overall phase arbitrariness

So next step is to deal with case where boundary conditions are not so obvious. $\delta(x)$ well and barrier.
V(x) = -a |δ(x)|  \quad (a > 0)

V(x) = 0 everywhere except \( V(0) = -a \) “\( \infty \)”

"strength" of the \( \delta \)-function well

\[
\text{Schrödinger Equation} \quad \frac{d^2\psi}{dx^2} = -\left( \frac{E + a\delta(x)}{E - V(x)} \right) \frac{2m}{\hbar^2} \psi
\]

Integrate:

\[
\lim_{\varepsilon \to 0} \int_{-\varepsilon}^{\varepsilon} \frac{d^2\psi}{dx^2} dx = -\lim_{\varepsilon \to 0} \left[ \int_{-\varepsilon}^{\varepsilon} \left( \frac{2mE}{\hbar^2} \psi(x) + \frac{2ma}{\hbar^2} \delta(x)\psi(x) \right) dx \right]
\]

LHS = \left[ \frac{d\psi}{dx} \right]_{x=\pm\varepsilon}^{} = \text{size of discontinuity in } \frac{d\psi}{dx} \text{ at } x = 0

RHS = \left[ 0 - \frac{2ma}{\hbar^2} \psi(0) \right]

because

\[ \frac{2mE}{\hbar^2} \psi(0) \]

is finite and integral over region of length \( 2\varepsilon \neq 0 \).

because, by the definition of a \( \delta \)-fn

\[ \int \delta(x)\psi(x) dx = \psi(0) \]

or, more generally

\[ \int_{-\infty}^{\infty} \delta(x \pm a)\psi(x) dx = \psi(a) \]
Since the potential has even symmetry wrt $x \rightarrow -x$, $\psi(x)$ must be even or odd (not a mixture) with respect to $x \rightarrow -x$, thus $\psi(x) = \pm \psi(-x)$. If $\psi(x)$ is even, there must be a cusp in $\psi(x)$ at $x = 0$

\[
\psi(x) \quad \begin{cases} 
\text{continuous} & \text{OR} \\
\text{not continuous} & \text{at } x = 0
\end{cases}
\]

\[
\frac{d\psi(\pm)}{dx} = \pm \frac{2ma}{\hbar^2} \psi(0)
\]

The new boundary condition

since there is $+$ reflection symmetry for an even $\psi(x)$

\[
\frac{d\psi(\pm)}{dx} = \mp \frac{ma}{\hbar^2} \psi(0)
\]

Now find the eigenfunctions and eigenvalues. Standard procedure: divide space into regions and match $\psi$ and $d\psi/dx$ across boundaries.
Let \( E < 0 \) \( \quad E = -|E| \)

\[
\psi_L = \psi_L = A_L e^{\rho x} + B_L e^{-\rho x} \quad \text{(8 unknowns, because A and B can be complex numbers)}
\]

\[
\psi_R = \psi_R = A_R e^{\rho x} + B_R e^{-\rho x}
\]

\[
\rho = \left[ \frac{|E|2m}{\hbar^2} \right]^{1/2}
\]

(THIS IS WHAT WE DO WHEN \( k \) WOULD BE IMAGINARY)

unknowns determined

\[
\psi(+\infty) = 0 \quad \Rightarrow \quad A_R = 0 \quad (2)
\]

\[
\psi(-\infty) = 0 \quad \Rightarrow \quad B_L = 0 \quad (2)
\]

\[
\psi_L(-\varepsilon) = \psi_R(+\varepsilon) = 0 \quad \Rightarrow \quad A_L = B_R \equiv A \quad (2)
\]

arbitrary phase

normalization

(1)

(8) Done!

\[
\frac{d\psi_R(\cdot)}{dx} = -\rho A e^{-\rho x} = -\frac{ma}{\hbar^2} \psi(0)
\]

required discontinuity in \( d\psi/dx \) at \( x = 0 \).

\[
\therefore \quad \rho = \frac{ma}{\hbar^2}
\]

\[
\frac{d\psi_L(\cdot)}{dx} = +\rho A e^{\rho x} = +\frac{ma}{\hbar^2} \psi(0)
\]

again \( \rho = \frac{ma}{\hbar^2} \).
Only one acceptable value of $\rho \rightarrow$ one value of $E < 0$

$$\rho = \frac{ma}{\hbar^2} \ \ |E| = \frac{\rho^2 \hbar^2}{2m} = \frac{ma^2}{2\hbar^2} = \pm E$$

$$E = \pm \frac{ma}{2\hbar^2}$$

Actually, the above solution was specifically for an even $\psi(x)$. What about odd $\psi(x)$? No calculation is needed. Why?

Normalization of $\psi$

$$1 = \int_{-\infty}^{\infty} |\psi|^2 \ dx$$

$$\psi_R = Ae^{-\max/h^2}$$

$$1 = 2 \int_0^{\infty} A f \ e^{-\left(2ma/h^2\right)x} \ dx = 2A \int_0^\infty \left( \frac{\hbar^2}{2ma} \right) f$$

$$A = \pm \left( \frac{ma}{\hbar^2} \right)^{1/2}$$

$$\psi_\delta = \pm \left( \frac{ma}{\hbar^2} \right)^{1/2} e^{-ma|x|/\hbar^2} \ \ \ \text{only one bound level, regardless of magnitude of } a$$

large $a$, narrower and taller $\psi$

There is a continuum of $\psi$’s possible for $E > 0$. Since the particle is free for $E > 0$, specific form of $\psi$ must reflect specific problem:

e.g., particle probability incident from $x < 0$ region. It is even more interesting to turn this into the simplest of all barrier scattering problems. See Non-Lecture pp. 2-8, 9, 10.
Nonlecture

Consider instead scattering off $V(x) = +\alpha\delta(x)$, $a > 0$

$V(x) = +\alpha\delta(x)$

\[
\psi_L = A_L e^{ikx} + B_L e^{-ikx} \quad k = \left(\frac{2mE}{\hbar^2}\right)^{1/2}
\]

\[
\psi_R = A_R e^{ikx} + B_R e^{-ikx}
\]

In this problem we have flux entering exclusively from left. The entering probability flux is $|A_L|^2$.

Two things can happen:

1. transmit through barrier $\propto |A_R|^2$
2. reflect at barrier $\propto |B_L|^2$

There is no way that $|B_R|^2$ can become different from 0. Why?

Our goal is to determine $|A_R|^2$ and $|B_L|^2$ vs. $E$

\[
\psi_L(0) = \psi_R(0)
\]

\[
A_L + B_L = A_R + B_R \quad \text{but } B_R = 0 \quad A_L + B_L = A_R
\]

\[
\left[ \frac{d\psi_R(0^+)}{dx} \pm \frac{d\psi_L(0^-)}{dx} \right] = \frac{2ma}{\hbar^2}\psi(0)
\]

\[
\frac{ikA_R \pm (ikA_L - ikB_L)}{h^2} = \frac{2ma}{h^2} A_R
\]

\[
\frac{ik(A_L + B_L) - ik(A_L - B_L)}{h^2} = \frac{2ma}{h^2} (A_L + B_L)
\]
\[ 2ikB_L = \frac{2ma}{h^2} (A_L + B_L) \]
\[ B_L \left( 2ik - \frac{2ma}{h^2} \right) = \frac{2ma}{h^2} A_L \]
\[ \frac{A_L}{B_L} = \frac{h^2}{2ma} \left( 2ik - \frac{2ma}{h^2} \right) = \frac{ikh^2}{ma} - 1 = \alpha \]
\[ \alpha + 1 = \frac{ikh^2}{ma} \]

\[ A_R = A_L + B_L = A_L \frac{B_L}{B_L} + B_L = \alpha B_L + B_L = B_L (\alpha + 1) \]

\[ A_R = B_L \left( \frac{ikh^2}{ma} \right) \]

Transmission is \[ T = \frac{|A_R|^2}{|A_L|^2} \]

Reflection is \[ R = \frac{|B_L|^2}{|A_L|^2} \]

What is \( T(E) \), \( R(E) \)?

\[ |A_R|^2 = |B_L|^2 \frac{k^2h^4}{m^2a^2} = |B_L|^2 \frac{2mE}{h^2} \frac{h^4}{m^2a^2} = |B_L|^2 \frac{2h^2E}{ma^2} \]

\[
\left( \frac{A_L}{B_L} \right) \left( \frac{A_L^*}{B_L^*} \right) = \left( \frac{ikh^2}{ma} - 1 \right) \left( -\frac{ikh^2}{ma} - 1 \right)
\]

\[ |A_L|^2 + |B_L|^2 = \frac{k^2h^4}{m^2a^2} + 1 = \frac{2h^2E + ma^2}{ma^2} \]

\[ R(E) = \frac{ma^2}{2h^2E + ma^2} = \left[ \frac{2h^2E}{ma^2} + 1 \right]^{-1} \]

\[ T(E) = \frac{2h^2E}{2h^2E + ma^2} = \left[ \frac{ma^2}{2h^2E} + 1 \right]^{-1} \]

\[ R(E) + T(E) = 1 \]

increasing to one as \( E \) increases
Note that: \( R(E) \) starts at 1 at \( E = 0 \) and goes to 0 at \( E \to \infty \) 

\[ T(E) \text{ starts at } 0 \text{ and increases monotonically to } 1 \text{ as } E \text{ increases.} \]

Note also that, at \( E = -\frac{ma^2}{2\hbar^2} \), \( R \to \infty \) as \( E \) approaches \(-ma^2/2\hbar^2\) from above and then changes sign as \( E \) passes through \(-ma^2/2\hbar^2\)!

This is the energy of the bound state in the \( \delta(x) \)-function well problem.

See CTDL Chapter 1 Problem #3b (page 87) for a related problem.