

5.73 Lecture #2

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Last Time: free particle $V(x)=V_0$ general solution
 $\psi = Ae^{ikx} + Be^{-ikx}$

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

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

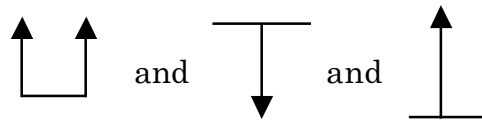
$$k = \left[(E - V_0) \frac{2m}{\hbar^2} \right]^{1/2} \quad \text{for } E \geq V_0$$

probability
distribution

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

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 (non-lecture)

What do we know about $\psi(x)$ for physically realistic $V(x)$?

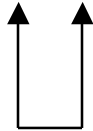
$\psi(\pm\infty) = ?$

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

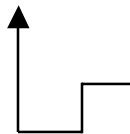
$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx$?

Continuity of ψ and $d\psi / dx$?

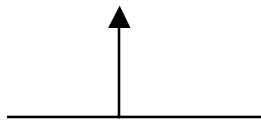
Computationally convenient potentials have steps and flat regions.



infinite step



finite step



infinitely high but infinitely thin step, "delta-function"

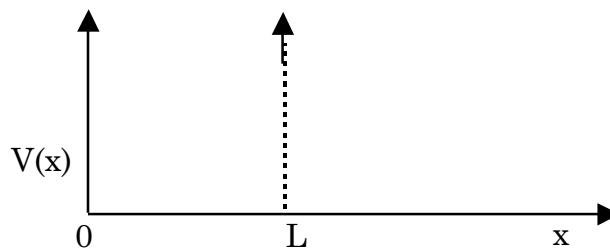
ψ continuous

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

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

More warm up exercises

1. Infinite box



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

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

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

$\psi(L) = 0 \Rightarrow kL = n\pi$

$n = 1, 2, \dots$ (why not $n = 0$?)

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recall $k^2 = (E - V_0) \frac{2m}{\hbar^2} = \frac{n^2 \pi^2}{L^2}$ $V_0 = 0$ here.

Insert $kL = n\pi$ boundary condition.

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

E_1

n = 0 would be empty box

E_n is integer multiple of common factor, E_1 .
Important for wavepackets!

∞ # of bound levels

normalization (P=1 for 1 particle in well)

$$1 = |D|^2 \int_0^L dx \sin^2(n\pi x / L)$$

\Rightarrow

$$|D| = (2 / L)^{1/2} \text{ because } \int_0^L \sin^2(n\pi x / L) dx = L / 2$$

$$\psi_n(x) = (2 / L)^{1/2} \sin(n\pi x / L)$$

$$D = (2 / L)^{1/2} \underbrace{e^{i\alpha}}_{\substack{\text{arbitrary} \\ \text{phase} \\ \text{factor}}}$$

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

left or right in x?

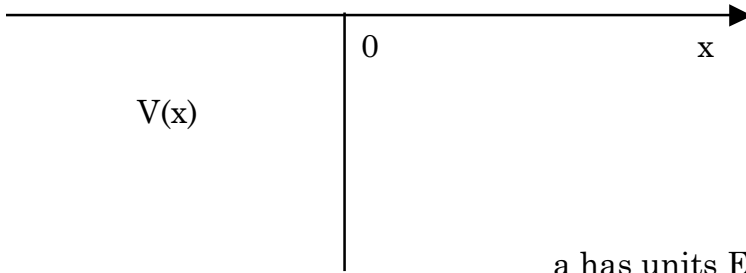
up or down in E?

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

Generalize to stepwise constant potentials: in each $V(x)=\text{constant}$ 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.



$$V(x) = -a|\delta(x)| \quad a > 0$$

$= 0$ everywhere except $V(0) = -a$ “ ∞ ”
 “strength” of the δ -function well

a has units Energy x Length
 (because, as we will see, $\delta(x)$ has
 units of reciprocal length)

Schrödinger
Equation

$$\frac{d^2\psi}{dx^2} = -\left(\frac{E + a\delta(x)}{E - V(x)}\right) \frac{2m}{\hbar^2} \psi$$

Integrate:

$$\lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{+\epsilon} \frac{d^2\psi}{dx^2} dx = -\lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{+\epsilon} dx \left(\frac{2mE}{\hbar^2} \psi(x) + \frac{2ma}{\hbar^2} \delta(x)\psi(x) \right)$$

$$\text{LHS} = \frac{d\psi}{dx} \Big|_{x=+\epsilon} \pm \frac{d\psi}{dx} \Big|_{x=-\epsilon} = \text{size of discontinuity in } \frac{d\psi}{dx} \text{ at } x = 0$$

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

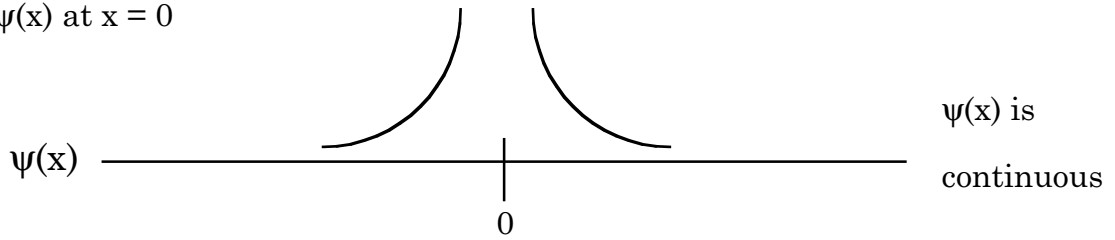
because $\frac{2mE}{\hbar^2} \psi(0)$
 is finite and integral
 is over region of
 length $2\epsilon \rightarrow 0$.

because, by the definition of a δ -fn
 $\int \delta(x)\psi(x)dx = \psi(0)$
 or, more generally
 $\int_{\pm\infty}^{\infty} \delta(x \pm a)\psi(x)dx = \psi(a)$

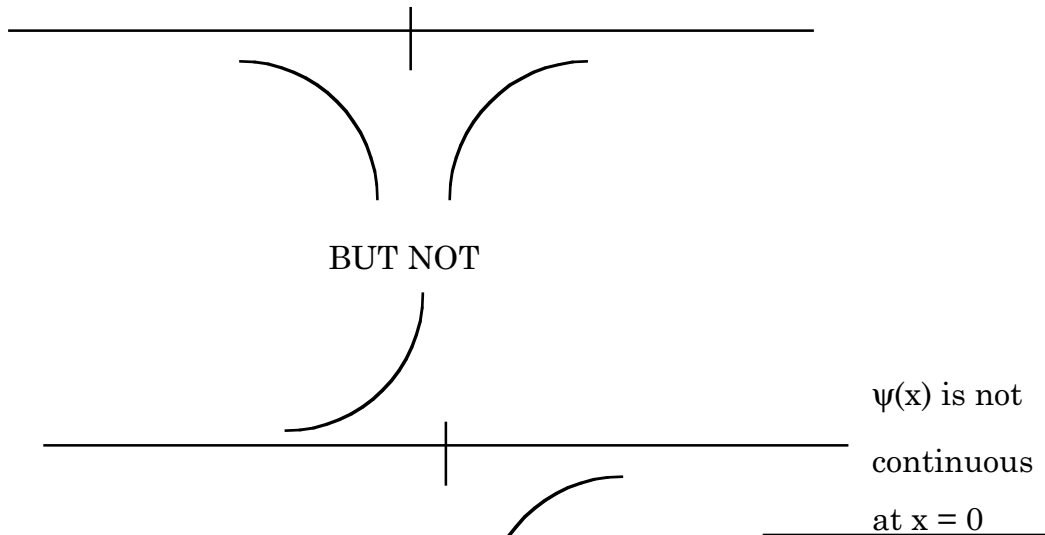
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Since the potential has even symmetry wrt $x \rightarrow -x$, $\psi(x)$ must be even or odd (not a mixture) with respect to $x \rightarrow -x$, thus $\psi(x) = \pm\psi(-x)$. If $\psi(x)$ is even, there must be a cusp in $\psi(x)$ at $x = 0$



OR



BUT NOT

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

The new boundary condition

So what happens when $\psi(x)$ is an odd function?

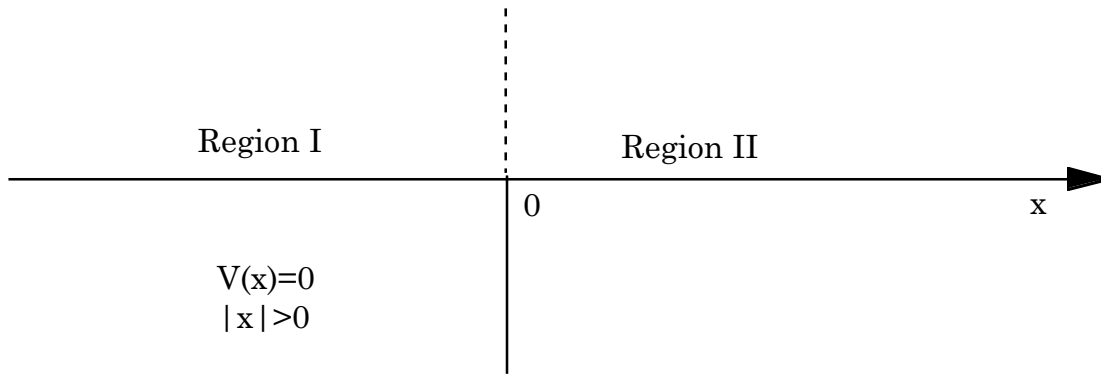
since there is + reflection symmetry for an even $\psi(x)$

$$\frac{d\psi(+)}{dx} = \pm \frac{d\psi(\pm)}{dx}$$

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

This is the δ -function joining condition for a symmetric potential.

Now find the eigenfunctions and eigenvalues. Standard procedure: divide space into regions and match ψ and $d\psi/dx$ across boundaries.



Let $E < 0$

$$E = -|E|$$

$$\psi_L = \psi_I = A_L e^{+\rho x} + B_L e^{-\rho x}$$

$$\psi_R = \psi_{II} = A_R e^{+\rho x} + B_R e^{-\rho x}$$

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

(8 unknowns, because A and B can be complex numbers)

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

unknowns determined

$$\psi(+\infty)=0 \quad \longrightarrow \quad \mathbf{A_R = 0} \quad (2)$$

$$\psi(-\infty)=0 \quad \longrightarrow \quad \mathbf{B_L = 0} \quad (2)$$

$$\psi_L(-\epsilon)=\psi_R(+\epsilon)0 \quad \longrightarrow \quad \mathbf{A_L = B_R \equiv A} \quad (2)$$

$$\psi_L = Ae^{\rho x}$$

$$\psi_R = Ae^{-\rho x}$$

$$\text{arbitrary phase} \quad (1)$$

$$\text{normalization} \quad (1)$$

$$(8) \quad \mathbf{Done!}$$

$$\frac{d\psi_R(+)}{dx} = -\rho A e^{-0} = \frac{-ma}{\hbar^2} \frac{\psi(0)}{A}$$

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

$$\therefore \rho = \frac{ma}{\hbar^2}$$

$$\frac{d\psi_L(-)}{dx} = +\rho A e^{+0} = \frac{+ma}{\hbar^2} \frac{\psi(0)}{A}$$

again $\rho = \frac{ma}{\hbar^2}$

Only one acceptable value of $\rho \rightarrow$ one value of $E < 0$

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

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

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

Normalization of ψ

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

$$\psi_R = Ae^{-ma|x|/\hbar^2}$$

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

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

see Gaussian Handout

$$\psi_{\delta} = \pm \left(\frac{ma}{\hbar^2} \right)^{1/2} e^{-ma|x|/\hbar^2}$$

only one bound level, regardless of magnitude of a

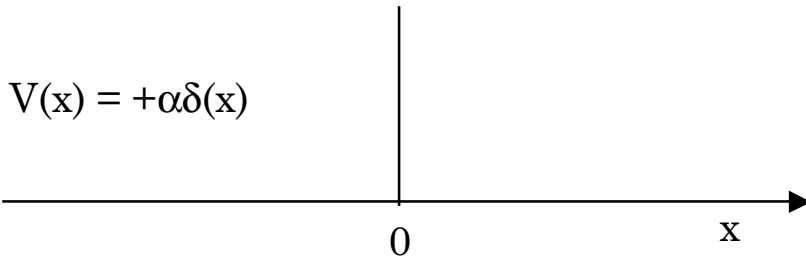
large a, narrower and taller ψ

There is a continuum of ψ 's possible for $E > 0$. Since the particle is free for $E > 0$, specific form of ψ 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 $V(x) = + a\delta(x)$ $a > 0$



$$\psi_L = A_L e^{ikx} + B_L e^{-ikx}$$

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

$$k = \left(\frac{2mE}{\hbar^2} \right)^{1/2}$$

In this problem assume that 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

$\psi_L(0) = \psi_R(0)$ continuity of ψ



$A_L + B_L = A_R + B_R$ but $B_R = 0$ $A_L + B_L = A_R$

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

$$ikA_R \pm (ikA_L - ikB_L) = \frac{2ma}{\hbar^2} A_R \quad \leftarrow \psi_R(0)$$

\uparrow $A_R = A_L + B_L$ \uparrow

$$ik(A_L + B_L) - ik(A_L - B_L) = \frac{2ma}{\hbar^2} (A_L + B_L)$$

\uparrow $\psi_L(0)$

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$$2ikB_L = \frac{2ma}{\hbar^2}(A_L + B_L)$$

$$B_L \left(2ik - \frac{2ma}{\hbar^2} \right) = \frac{2ma}{\hbar^2} A_L$$

$$\frac{A_L}{B_L} = \frac{\hbar^2}{2ma} \left(2ik - \frac{2ma}{\hbar^2} \right) = \frac{ik\hbar^2}{ma} - 1 \equiv \alpha$$

$$\alpha + 1 = \frac{ik\hbar^2}{ma}$$

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

$$A_R = B_L \left(\frac{ik\hbar^2}{ma} \right)$$

$$\alpha = A_L/B_L$$

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)?

$$|A_R|^2 = |B_L|^2 \frac{k^2 \hbar^4}{m^2 a^2} = |B_L|^2 \frac{2mE}{\hbar^2} \frac{\hbar^4}{m^2 a^2} = |B_L|^2 \frac{2\hbar^2 E}{ma^2}$$

$$\left(\frac{A_L}{B_L} \right) \left(\frac{A_L}{B_L} \right)^* = \left(\frac{ik\hbar^2}{ma} - 1 \right) \left(-\frac{ik\hbar^2}{ma} - 1 \right)$$

$$\frac{|A_L|^2}{|B_L|^2} = \frac{k^2 \hbar^4}{m^2 a^2} + 1 = \frac{2\hbar^2 E + ma^2}{ma^2}$$

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

decreasing to zero as E increases

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

increasing to one as E increases

$$R(E) + T(E) = 1$$

Note that: $R(E)$ starts at 1 at $E = 0$ and goes to 0 at $E \rightarrow \infty$

$T(E)$ starts at 0 and increases monotonically to 1 as E increases.

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

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