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

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

A,B are complex constants, determined by "boundary conditions"

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

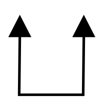
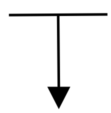
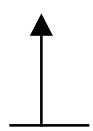
$$k = \left[(E - V_0)\frac{2m}{\hbar^2}\right]^{1/2} \qquad \text{for } E \geq V_0$$

probability distribution

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

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

TODAY

 and  and 

1. infinite box
2. δ(x) well
3. δ(x) barrier

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

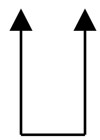
$\psi(\pm\infty) = ?$

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

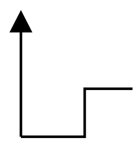
$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx?$

Continuity of ψ and $d\psi/dx$?

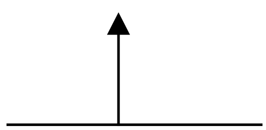
Computationally convenient potentials have steps and flat regions.



infinite step



finite step



infinitely high but infinitely thin step,“δ-function”

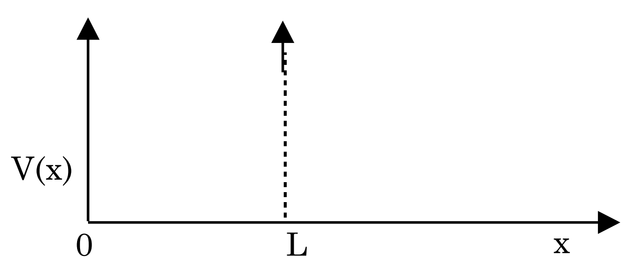
ψ continuous

$\frac{d\psi}{dx}, \frac{d^2\psi}{dx^2}$ 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



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

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

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

$\psi(L) = 0 \Rightarrow kL = n\pi \qquad n = 1,2,\ldots \qquad$ (why not n = 0?)

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

Insert $kL = n\pi$ boundary condition.

$$E_n = n^2\frac{\hbar^2\pi^2}{2mL^2} = n^2\underbrace{\left[\frac{h^2}{8mL^2}\right]}_{E_1}$$

n = 0 would be empty box

∞ # of bound levels

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

normalization (P=1 for 1 particle in well)

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

$$\psi_n(x) = (2/L)^{1/2}\sin(n\pi x) \qquad D = (2/L)^{1/2}\underbrace{e^{i\alpha}}_{\substack{\text{arbitrary}\\ \text{phase}\\ \text{factor}}}$$

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

left or right in x?

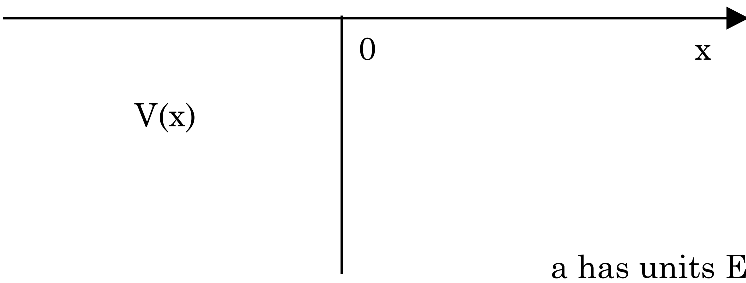
up or down in E?

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

Generalize to stepwise constant potentials: in each V(x)=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.



$V(x) = -a\,\boxed{\delta(x)}$ $\quad a > 0$

= 0 everywhere except V(0) = –a "∞"

"strength" of the δ-function well

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

Schrödinger Equation $\quad \dfrac{d^2\psi}{dx^2} = -\left(\underbrace{(E + a\delta(x))}_{E-V(x)}\right)\dfrac{2m}{\hbar^2}\psi$

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

$$\text{LHS} = \left.\frac{d\psi}{dx}\right|_{x=+\varepsilon} \pm \left.\frac{d\psi}{dx}\right|_{x=-\varepsilon} =$$ size of discontinuity in $\dfrac{d\psi}{dx}$ at x = 0

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

because $\dfrac{2mE}{\hbar^2}\psi(0)$ is finite and integral over region of length 2ε ♦ 0.

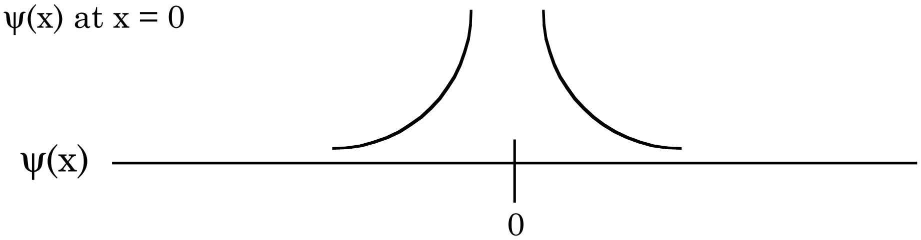
because, by the definition of a δ–fn

$$\int \delta(x)\psi(x)dx = \psi(0)$$

or, more generally

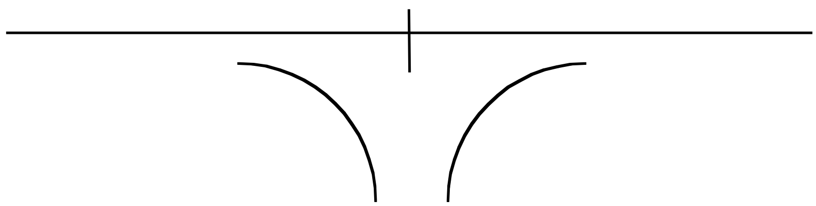
$$\int_{\pm\infty}^{\infty}\delta(x \pm a)\psi(x)dx = \psi(a)$$

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

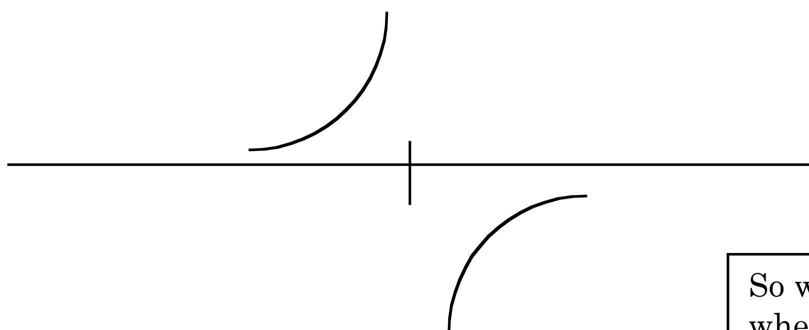


$\psi(x)$ is continuous

OR



BUT NOT



$\psi(x)$ is not continuous at $x = 0$

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

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

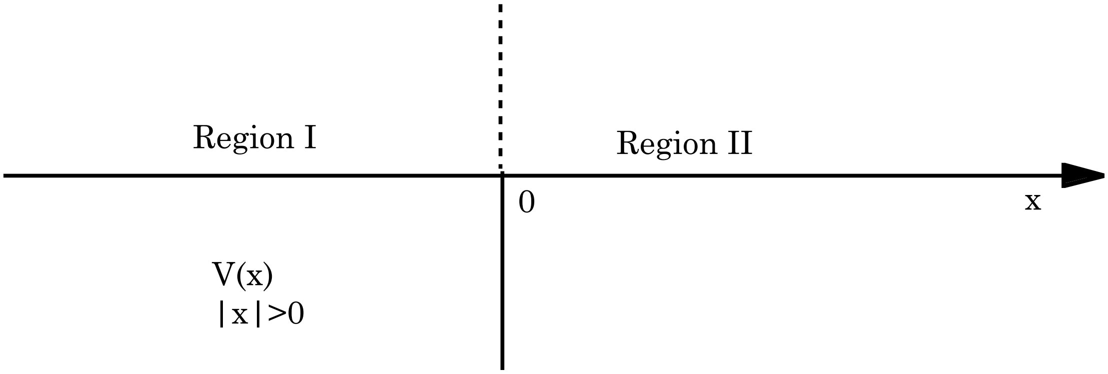
The new boundary condition

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

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

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

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



Let $E < 0$ $\quad E = -|E|$

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

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

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

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

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

			unknowns determined	
$\psi(+\infty)=0$	$\longrightarrow$	**$A_R = 0$**	**(2)**	
$\psi(-\infty)=0$	$\longrightarrow$	**$B_L = 0$**	**(2)**	$\psi_L = Ae^{\rho x}$
$\psi_L(-\varepsilon)=\psi_R(+\varepsilon)0$	$\longrightarrow$	**$A_L = B_R \equiv A$**	**(2)**	$\psi_R = Ae^{-\rho x}$
	arbitrary phase		**(1)**	
	normalization		**<u>(1)</u>**	
			(8)	**Done!**

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

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

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

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

again $\quad \rho = \dfrac{ma}{\hbar^2}$

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

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

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

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

Normalization of ψ

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

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

$$1 = 2\int_0^{\infty} |A|^2\, e^{-\left(2ma/\hbar^2\right)x} dx = 2|A|^2 \underbrace{\left(\frac{\hbar^2}{2ma}\right)}_{\text{see Gaussian Handout}}$$

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

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

only one bound level, regardless of magnitude of a

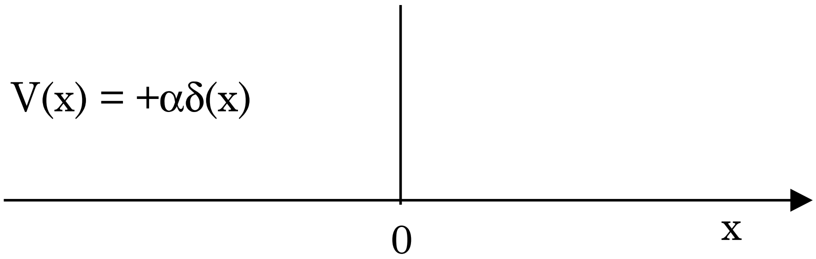
large a, narrower and taller ψ

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 $V(x) = +\alpha\delta(x)$ $\quad\quad$ $a > 0$



$$\psi_L = A_L e^{ikx} + B_L e^{-ikx} \qquad k = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$$
$$\psi_R = A_R e^{ikx} + B_R e^{-ikx}$$

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 $\quad \propto |A_R|^2$
2. reflect at barrier $\quad \propto |B_L|^2$

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

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

$$\Downarrow$$

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

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

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

$A_R = A_L + B_L$

$$ik(A_L + B_L) - ik(A_L - B_L) = \frac{2ma}{\hbar^2}\underbrace{(A_L + B_L)}_{\psi_L(0)}$$

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

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

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

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

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

$\alpha = A_L/B_L$

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

Transmission is $\quad T = \dfrac{|A_R|^2}{|A_L|^2}$

Reflection is $\quad R = \dfrac{|B_L|^2}{|A_L|^2}$

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

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

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

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

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

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

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

Note also that, at $\boxed{E = -\frac{ma^2}{2\hbar^2}}$ $R \to \infty$ 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 δ(x)-function well problem.

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