Infinite Box, $\delta(x)$ Well, $\delta(x)$ Barrier.

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

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

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

$k = \frac{p}{\hbar}$ (from e^{ikx}, an eigenfunction of $\hat{p}$ for a free particle, and the real number, $\hbar k = p$, is the eigenvalue of $\hat{p}$)

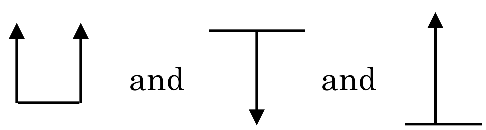
$$k = \left[\left(E - V_0\right)\frac{2m}{\hbar^2}\right]^{1/2} \quad \text{for } E \geq V_0$$

probability distribution

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

only get wiggly stuff when ψ contains a superposition of 2 or more different values of k are superimposed. In this special case we had the two values of k: $+k$ and $-k$.

TODAY



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

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

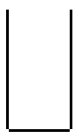
$\psi(\pm\infty) = ?$

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

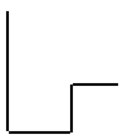
$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx?$

Continuity of ψ and $d\psi/dx$?

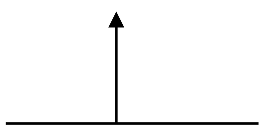
Computationally convenient potentials have steps and flat regions.



infinite step



finite step



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

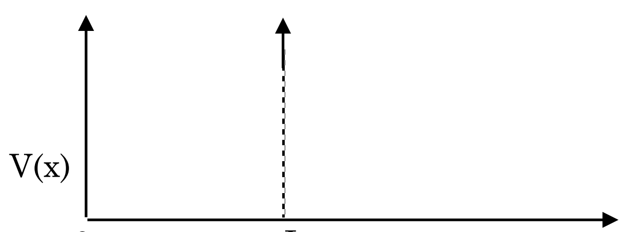
ψ continuous

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

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

<u>More warm up exercises</u>

1. Infinite box



$$\psi(x) = Ae^{ikx} + Be^{-ikx} = C\cos kx + D\sin kx \qquad [C = A + B, D = iA - iB]$$

Where do these 2 equations come from? Be sure you can derive (and never forget) these 2 equations for C and D.

Boundary conditions:

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

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

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

Insert $kL = n\pi$ boundary condition

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

∞ # of bound levels

n = 0 would be empty box!

E_n is integer multiple of common factor, E_1. Important for many wavepacket problems!

normalization (P=1 for 1 particle in well)

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

because $\int_0^L \sin^2(n\pi x/L)dx = L/2$

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

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

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

left or right in x?

up or down in E?

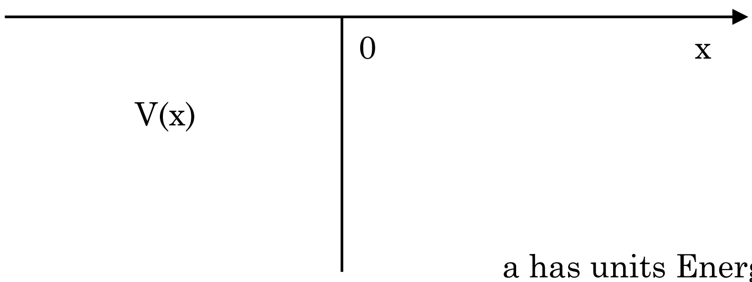
There is always a short-cut. A picture is often more informative than equations.

Infinite well was easy: 2 boundary conditions plus a 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.



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

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

$\delta(x)$ = 0 everywhere except V(0) = –a "∞", a is the "strength" of the δ-function well

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

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

$$LHS = \left.\frac{d\psi}{dx}\right|_{x=+\varepsilon} - \left.\frac{d\psi}{dx}\right|_{x=-\varepsilon} =$$

size of discontinuity in $\frac{d\psi}{dx}$ at x = 0

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

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

because, by the definition of a δ–fn,

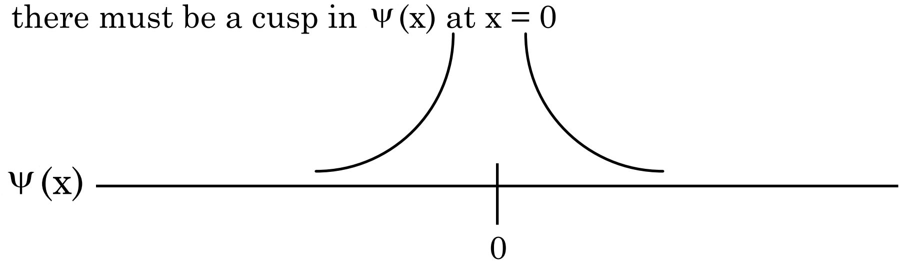
$$\int \delta(x)\psi(x)dx = \psi(0)$$

or, more generally

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

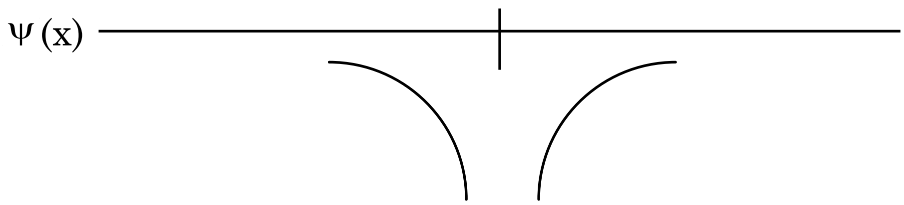
This is a really important derivation. You will want to remember it!

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



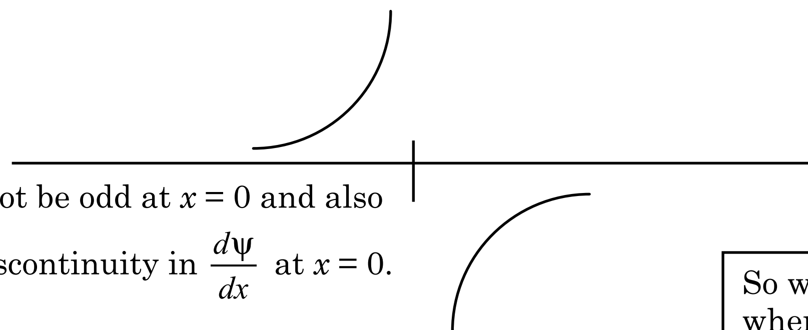
$\psi(x)$ is continuous

OR



$\psi(x)$ is continuous

BUT NOT



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

$\psi(x)$ cannot be odd at $x = 0$ and also have a discontinuity in $\frac{d\psi}{dx}$ at $x = 0$.

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

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

Thus we have a new connection condition on $\frac{d\psi}{dx}$

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

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

$$\boxed{\begin{aligned} \frac{d\psi(\pm)}{dx} &= \mp\frac{ma}{\hbar^2}\psi(0) \\ \frac{d\psi(+)}{dx} - \frac{d\psi(-)}{dx} &= -\frac{2ma}{\hbar^2}\psi(0) \end{aligned}}$$

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.

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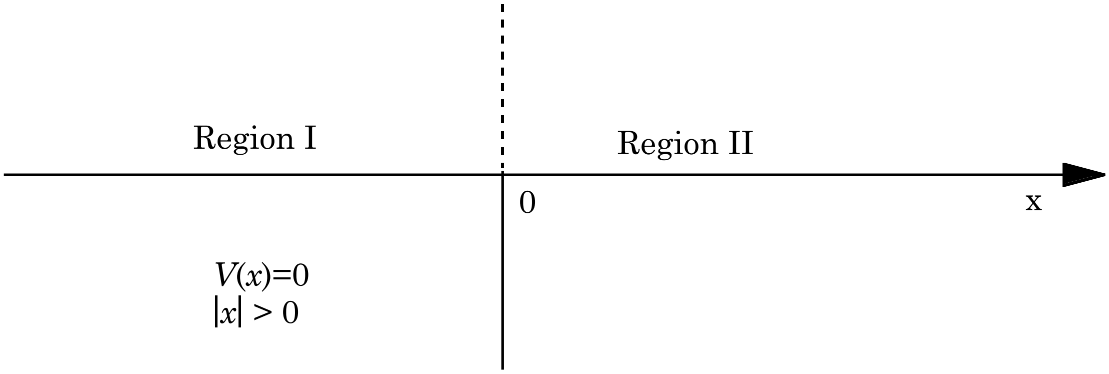


Let E < 0 $\quad E = -|E|$

$$\psi_L \equiv \psi_{\mathrm{I}} = A_L e^{+\kappa x} + B_L e^{-\kappa x}$$

$$\psi_R \equiv \psi_{\mathrm{II}} = A_R e^{+\kappa x} + B_R e^{-\kappa x}$$

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

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

$$\kappa = ik$$

(THIS IS WHAT WE ALWAYS DO WHEN k IS IMAGINARY)

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

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

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

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

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

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

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

$$\kappa = \frac{ma}{\hbar^2}$$

$$|E| = \frac{\kappa^2\hbar^2}{2m} = \frac{ma^2}{2\hbar^2} = -E$$

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

Actually, the above solution was specifically for an even $\psi(x)$. What about an odd $\psi(x)$ for a $V(x)$ with a $\delta(x)$ at x = 0? *No calculation is needed.* Why?

Normalization of ψ

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

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

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

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

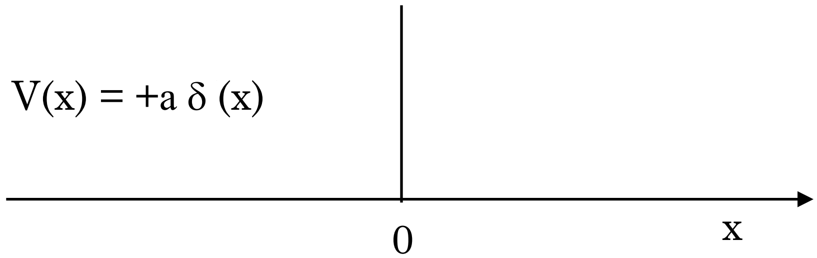
large a, narrower and taller ψ

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



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

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

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

In this problem let's assume that we have flux entering exclusively from the 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? (Hint: where does the flux enter the system and in what direction is it flowing?)

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

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

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

discontinuity of $\frac{d\psi}{dx}$ at δ-function

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

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

$A_R = A_L + B_L$

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

$(A_L + B_L)$: $\psi_L(0)$

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

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

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

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

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

$\alpha = A_L/B_L$

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

Transmission is $\mathrm{T} = \frac{|A_R|^2}{|A_L|^2}$: $\frac{(\text{moving to right in R region})}{(\text{incident from left in L region})}$

Reflection is $\mathrm{R} = \frac{|B_L|^2}{|A_L|^2}$: $\frac{(\text{moving to left in L region})}{(\text{incident from left in L region})}$

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

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

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

$$\frac{|A_L|^2}{|B_L|^2} = \frac{k^2\hbar^4}{m^2a^2} + 1 = \frac{2\hbar^2E + ma^2}{ma^2} \qquad \left[k = \left(\frac{2mE}{\hbar^2}\right)^{1/2}\right]$$

$$R(E) = \frac{ma^2}{2\hbar^2E + ma^2} = \left[\frac{2\hbar^2E}{ma^2} + 1\right]^{-1}$$ 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 extending the equations for $R(E)$ and $T(E)$ to $E < 0$, we see 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 $-ma^2/2\hbar^2$!

<u>This is the energy</u> of the bound state in the δ (x)-function well problem.

↓

This tells you that something special happens when you "extend" the scattering calculation to scattering off a V(x) at the energy of a bound state. This is strange because it is difficult to imagine scattering at E < 0.

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