PH253
9 Feb 2010
deBrog./Schr.

De Broglie: take $\lambda \leftrightarrow p$ relationship for photon as general

- no evidence at the time
- wave-like properties of e^- by diffraction soon after!

$$\lambda = \frac{h}{p} = \frac{h}{\gamma m v} \simeq \frac{h}{mv}$$

$\boxed{\text{massive particles}}$: $p = \gamma m v \Rightarrow \boxed{\frac{v}{c} = \frac{1}{\sqrt{1+\left(\frac{mc}{p}\right)^2}}}$

if $p \gg mc$, $v \approx c$

relativistic ... photon-like

if $p \ll mc$, $v \ll c$

non-relativistic

for photons, observing $v = c$ over many orders

e.g. UV ~ nm to radio ~ m

$\Rightarrow$ photon mass $\lesssim 10^{-44}$ g

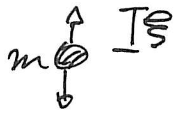
$\boxed{\text{photon = special case}}$ with $m \simeq 0$

- what about a particle with a non-zero mass?
- rest frame, $m \neq 0$

$$\Rightarrow \boxed{hf_0 = mc^2} \quad \text{via } E = hf$$

rest mass

- if we associate a vibration or wave with the particle ... what is p? λ?
- vibration implied is



$\xi_0 \sim \sin(2\pi f_0 t_0)$ in particle's rest frame

Simple vibration

- Lab frame? time dilation ...

$t_0 = \gamma\left(t - \frac{vx}{c^2}\right)$ $\quad$ t = our time
x = our dist to particle
v = particle rel. velocity

$\Rightarrow \quad \xi(x,t) = \sin\left[2\pi f_0 \gamma\left(t - \frac{vx}{c^2}\right)\right]$

or $\quad \xi(x,t) = \sin\left[2\pi f\left(t - \frac{x}{W}\right)\right]$

a wave with $\boxed{\text{freq. } f = \gamma f_0}$

$\boxed{\text{"velocity" } W = \frac{c^2}{v}}$ just from math. analogy

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Vibration in rest frame $\longleftrightarrow$ wave in our frame?!

energy in our frame? $hf = \gamma h f_0 = E = \gamma mc^2$

wavelength we see? ratio of speed to freq

$$\lambda = \frac{W}{f} = \frac{c^2}{v\gamma f_0} = \frac{hc^2}{v} \cdot \frac{1}{\gamma h f_0} = \frac{hc^2}{v\gamma mc^2} = \frac{h}{\gamma mv} = \frac{h}{p}$$

- plausibility of de Broglie relationship
  - based on inherent oscillations of matter
  - relativity

? how does this relate to particle velocity

? consistency of viewpoints?

? why is wave velocity greater than c?

$$\boxed{W = \frac{c^2}{v} > c}$$ screws up this idea?

Problem there are different wave velocities!

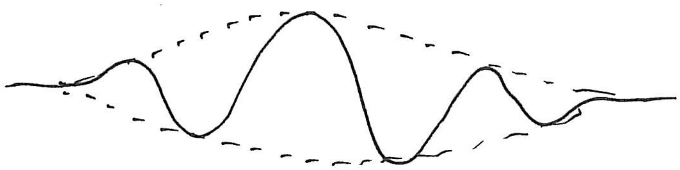
speed of a pulse ≠ speed of continuous wave!

speed of individual peaks

vs. speed of wave "packets"?

e.g. water waves!

individual wave amplitudes vs. group of waves



- crests & troughs within pulse move faster than group!

group → "group velocity" v_g

one crest → "phase velocity"

adding 2 sine waves diff frequencies

$\boxed{\text{take a simple wave}}$ $y(x,t) = A\sin(kx - \omega t)$

recall $k = \frac{2\pi}{\lambda}$ $\quad \omega = 2\pi f$

$\boxed{\text{Combine 2 slightly displaced waves}}$

$$y_1 = A\sin(kx - \omega t)$$

$$y_2 = A\sin[(k+\Delta k)x - (\omega + \Delta\omega)t]$$

individual phase velocities for clarity, call them v_p

$$v_{p1} = \frac{\omega}{k} \qquad v_{p2} = \frac{\omega + \Delta\omega}{k + \Delta k}$$

- if $\Delta\omega \ll \omega$ (and $\Delta k \ll k$) $v_{p1} \approx v_{p2}$
- combined disturbance (use some trig ...)

$$y = y_1 + y_2 = 2A \underbrace{\sin\left[\left(k+\tfrac{1}{2}\Delta k\right)x - \left(\omega + \tfrac{1}{2}\Delta\omega\right)t\right]}_{\text{main waveform}} \underbrace{\cos\left[\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right]}_{\text{modulation of waveform "envelope"}}$$

- modulation envelope moves at GROUP velocity
- as with any wave: $v = \left(\dfrac{x \text{ coeff}}{t \text{ coeff}}\right)$

$$\Rightarrow \boxed{v_g = \frac{\Delta\omega}{\Delta k}} \quad \xrightarrow[\Delta f \to 0]{\text{tiny diffs in freq}} \quad \boxed{v_g = \frac{d\omega}{dk}}$$

- knowledge of $\omega(k) \rightarrow$ group velocity
- this is the velocity of $\begin{cases} \text{energy transfer} \\ \text{matter transfer} \\ \text{information} \end{cases}$

$\boxed{\text{So:}}$ phase velocity: $v_{ph} = \dfrac{\omega}{k}$ indiv. crests

group velocity: $v_g = \dfrac{d\omega}{dk}$ clumps/packets/modulation

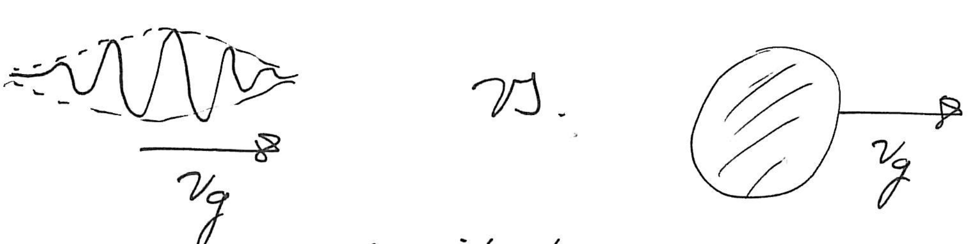
$\boxed{\text{Applied to de Broglie?}}$

$$\omega = 2\pi f = \frac{\omega_0}{\sqrt{1-v^2/c^2}} \qquad k = \frac{2\pi}{\lambda} = \frac{v\,\omega_0}{c^2\sqrt{1-v^2/c^2}}$$

$$\boxed{v_{ph} = \frac{\omega}{k} = \frac{c^2}{v^2}}$$

$$\boxed{v_g = \frac{d\omega}{dk} = v}$$ as you'll show in HW!

group velocity of de Broglie wave $\parallel$ velocity of associated particle!



<u>Consistent</u>

- Matter still travels with $v < c$
- wave $\leftrightarrow$ particle transition consistent

$\boxed{\text{more things:}}$ relation to KE?

$$K = p^2/2m \longrightarrow p = \sqrt{2mK}$$

$$\Rightarrow \boxed{\lambda = \frac{h}{\sqrt{2mK}}} \qquad K\uparrow,\ \lambda\downarrow$$

uncertainty

$$\Delta x \geq \frac{\lambda_c}{4\pi}$$

natural limit of localization

further: $E^2 = c^2p^2 + m^2c^4 = (K + mc^2)^2$

$$\Rightarrow \quad cp = \sqrt{2mc^2K + K^2}$$

$$\Rightarrow \boxed{\lambda = \frac{hc}{\sqrt{2mc^2K + K^2}}}$$

- at very high K $(K \gg mc^2)$ scale for rel to set in

$$\boxed{\lambda \approx \frac{hc}{K}} \quad \text{ultra-relativistic}$$

- recall relevant energy scale is mc^2 for a particle

$$\boxed{\lambda = \frac{(h/mc)}{\sqrt{2\left(\frac{K}{mc^2}\right) + \left(\frac{K}{mc^2}\right)^2}}} \quad \text{or} \quad \boxed{\frac{\lambda}{\lambda_c} = \frac{1}{\sqrt{2\left(\frac{K}{mc^2}\right) + \left(\frac{K}{mc^2}\right)^2}}}$$

$\lambda_c = \left(\frac{h}{mc}\right)$ = Compton wavelength for the particle! (m = particle mass; e^- special case)

- $K \ll mc^2$ "classical" $\lambda \sim \sqrt{\frac{1}{K}}$
- $K \gg mc^2$ "relativistic" $\lambda \sim 1/K$
- $\Delta X < \lambda_c$ probe $< \lambda_c$ impossible to localize particle!

$\boxed{\text{How to do mechanics w/ Matter waves?}}$

- we need a new wave equation! [Today: motivate "Tomorrow": solutions]
- need so far:

$$\lambda = \frac{h}{p}, \quad E = hf$$

- aux: $\boxed{k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h}}$ $\boxed{\omega = 2\pi f = \frac{2\pi E}{h}}$

$$\Rightarrow \quad \underline{E = hf = \hbar\omega}, \quad \underline{p = \hbar k}$$

$\boxed{\text{Requirements?}}$ obey energy conservation ... classically?

$$E = \frac{p^2}{2m} + U(x) \underset{\text{defs}}{\Rightarrow} \boxed{\hbar\omega = \frac{\hbar^2 k^2}{2m} + U(x)}$$

(does NOT apply to photons, since $m = 0$ and $v = c$)
NOT a problem, we know photon total $E = hf$

$\boxed{\text{Also}}$ LINEAR in time $\Rightarrow$ obey superposition!
1st order in time

Quantum: need to calculate probability distribution
—or— wave intensity

- take a free particle, $U(x) = 0$ (purely kinetic energy)
  $\Rightarrow$ specific E, p
- classical wave analogy $\Rightarrow$ specific ω, k

$$y(x,t) = A\sin(kx - \omega t)$$

basic equation governing classical wave

$$\boxed{\underbrace{\frac{\partial^2 y}{\partial x^2}}_{\text{"spread"}} = \frac{1}{v_g^2}\underbrace{\frac{\partial^2 y}{\partial t^2}}_{\text{accel.}}}$$

we know the general solutions are

$$y = f(x+vt) \pm g(x-vt)$$

for our eqn,

$$\boxed{\begin{aligned}\frac{\partial y}{\partial x} &= kA\cos(kx-\omega t)\\ \frac{\partial y}{\partial t} &= -\omega A\cos(kx-\omega t)\end{aligned}}$$

or $$\boxed{\frac{\partial y}{\partial x} = -\left(\frac{k}{\omega}\right)\frac{\partial y}{\partial t} = -\left(\frac{1}{v_g}\right)\frac{\partial y}{\partial t}}$$

So our wave obeys a 1st order Diff eq

$$\frac{\partial y}{\partial x} = \pm\left(\frac{1}{v_g}\right)\left(\frac{\partial y}{\partial t}\right)$$

- necessary for quantum approach!

  $\boxed{\text{first order in time}} \rightarrow$ unique physical solns

- what will work & satisfy quantum postulates?

  $k = P/\hbar\ , \quad \omega = E/\hbar$

Say $\Psi = A\sin(kx-\omega t)$ $\boxed{\text{now notice:}}$

$$\frac{\partial^2\Psi}{\partial x^2} = -k^2 A\sin(kx-\omega t)$$

$$\frac{\partial\Psi}{\partial t} = -\omega A\cos(kx-\omega t)$$

Prop, except...

~~classical~~ free particle : $\boxed{\omega = \frac{\hbar k^2}{2m} \Rightarrow \frac{\partial\Psi}{\partial t} = -\frac{\hbar k^2}{2m} A\cos(kx-\omega t)}$

WOULD get this from above... $\boxed{\frac{\partial\Psi}{\partial t} \propto \frac{\partial^2\Psi}{\partial x^2}}$

$\boxed{\text{except}}$ sine vs cosine!

$$\frac{\partial^2\Psi}{\partial x^2} \overset{?}{=} \frac{2m}{\hbar}\frac{\partial\Psi}{\partial t}$$

- 1st order in time, OK
- how to fix?

! represent quantum waves by complex exponentials !

$$\boxed{\Psi(x,t) = A e^{i(kx-\omega t)}}$$

classical : take real part $\rightarrow$ phys soln

quantum : only $|\Psi|^2$ observable, Ψ MUST be complex to be consistent

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as we said before: quantum waves need to be complex to capture interference ... wave fn itself not observable

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now try :

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 A e^{i(kx-\omega t)} = -\frac{p^2}{\hbar^2} \Psi(x,t)$$

$$\frac{\partial \Psi}{\partial t} = -i\omega A e^{i(kx-\omega t)} = \frac{-iE}{\hbar} \Psi$$

Combining :

$$\boxed{\frac{\partial^2 \Psi}{\partial x^2} = -\left(\frac{2mE}{\hbar^2}\right)\Psi = -i\left(\frac{2m}{\hbar}\right)\frac{\partial \Psi}{\partial t}}$$

Schrodinger eqn for free particle! i.e. $U(x)=0$

- time & spatial evolution of "matter wave"

$\Rightarrow$ probability of finding a particle at $x \propto |\Psi|^2$

What if we also have potential energy?

$p^2 = 2m(E-V) = \hbar^2 k^2$ Only MOD required!

$$\Rightarrow \quad \frac{\partial^2 \psi}{\partial x^2} = -\frac{2m}{\hbar^2}(E-V)\psi = -i\left(\frac{2m}{\hbar}\right)\frac{\partial \psi}{\partial t} + \frac{2m}{\hbar^2}V\psi$$

$\boxed{\text{2 forms}}$

$$\Rightarrow \quad \boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = E\psi \qquad \text{time-indep}}$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar\frac{\partial \psi}{\partial t} \qquad \text{time-dep}}$$

Schrödinger eqn

Will NOT solve these a lot...

$\boxed{\text{Properties}}$ of note

1) LINEARITY: sum of any 2 solns also a soln!
   $\Rightarrow$ Superposition; key & basic wave property
   consistency w/ classical phys!

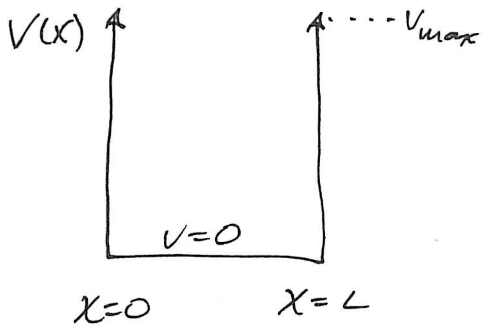
2) ψ is a probability amplitude as in our slit expt

3) it really WORKS

General procedure

- need $U(x)$ potential function
- need boundary conditions

e.g. $\boxed{\text{particle in a box}}$ - like Black body



- could be an e^- in between 2 negative plates
- 1st approx: VERY deep cannot escape - "trapped" $V_{max} \to \infty$

$$\boxed{\text{potential } V(x) = \begin{cases} 0 & 0<x<L \\ \infty & x>L,\ x<0 \end{cases}}$$

Boundary conditions?

- wave can't penetrate boundary! "turning points"

$$\psi(0) = \psi(L) = 0$$

- inside "box" purely kinetic! $V=0$

$$\Rightarrow \boxed{E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}}$$ no potential E (can set to zero)

$$\Rightarrow \frac{d^2\psi}{dx^2} = -\left(\frac{2mE}{\hbar^2}\right)\psi = -k^2\psi \quad \text{with } k = \pm\frac{\sqrt{2mE}}{\hbar}$$

- Basically like a held string!
- satisfied by $\psi(x) = e^{\pm ikx}$

or general $\psi(x) = C_1 e^{ikx} + C_2 e^{-ikx}$ $\quad |k| = \frac{\sqrt{2mE}}{\hbar}$

$\boxed{C_1 \,\&\, C_2 ?}$ BC's!

$\psi(0) = 0 \quad \Rightarrow \boxed{C_1 = -C_2}$

$\psi(x) = C_1 \left(e^{ikx} - e^{-ikx}\right)$

$\psi(L) = 0 \quad \Rightarrow \quad \sin(kL) = 0 \quad \Rightarrow \boxed{kL = n\pi}$

wave has <u>discrete</u> k (or λ)

$$\boxed{k_n = \frac{n\pi}{L} \quad n = 1, 2, 3, \ldots}$$ <u>n = mode</u> or <u>harmonic</u>

as w/ EM wave in box!

implies discrete energies! $\boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 h^2}{8mL^2}}$

thus $\psi(x) = \begin{cases} A_n \sin\left(\frac{n\pi x}{L}\right) e^{-(E_n/\hbar)t} & 0 < x < L \\ 0 & x > L,\ x < 0 \end{cases}$

<u>Schrodinger + BC's</u> $\Rightarrow$ Quantized energy! full circle :)

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2}$$ Schrodinger for free particle

- most gen soln: $\Psi(x,t) = \underbrace{\frac{1}{\sqrt{2\pi\hbar}}}_{\text{from where?}} \int dp\, \phi(p)\, e^{i[px-(p^2/2m)t]/\hbar}$

  $\phi(p)$ function of momentum (Fourier xform...)

- 1st order in time ⇒ initial value of $\Psi(x,0) \rightarrow$ all other times

- rewrite as a program (w) sees it:

$$\boxed{\Psi(x,t+\Delta t) = \Psi(x,t) + \left[\frac{i\hbar}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2}\right]\Delta t}$$

using $\frac{\partial \Psi}{\partial t} \approx \frac{\Psi(t+\Delta t)-\Psi(t)}{\Delta t}$ for discrete time steps

- given $\Psi(x,0)$, $\phi(p)$ can be found from gen soln

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi\hbar}}\int dp\, \phi(p)\, e^{ipx/\hbar}$$

$\phi(p)$: fn of momentum

- no "uncertainty" here yet: deterministic!
  initial conditions?
  properties of actual solns...

General remarks

1) Ψ is complex! $|\Psi(x,t)|$ large where the particle is supposed to be

$\Rightarrow |\Psi|^2 = \Psi^* \Psi$ ... mult. complex conjugates

2) interpretation of Ψ? $|\Psi(x,t)|^2$ is a probability density

$$\boxed{P(x,t)\,dx = |\Psi(x,t)|^2 dx}$$ prob particle is in $[x, x+dx]$ at time t

analogy w/ intensity of EM waves, $I \propto |E|^2$

for consistency, $P=1$ that particle is *somewhere*

i.e. $\displaystyle\int_{-\infty}^{\infty} P(x,t)\,dx = 1$ "normalization" ⇒ overall constants

so probability that particle lies in $[a,b] \in x$

$$P_{ab}(t) = \int_a^b P(x,t)\,dx = \int_a^b |\Psi(x,t)|^2 dx$$

3) phase of Ψ is important even though we find $|\Psi|^2$

since Schr. is linear, if Ψ_1 and Ψ_2 are solns

so is $\Psi_3 = a\Psi_1 + b\Psi_2$

$|\Psi_3|^2 \neq |\Psi_1|^2 + |\Psi_2|^2$ interference!

Same as adding $\vec{E}_1 + \vec{E}_2$ EM waves & finding $I = |E|^2$

4) measurements of a physical variable may vary due to uncertainty BUT an "expectation value" can be assigned

e.g. position : you'll get scatter around a mean $\langle x \rangle$

how to calculate? operators for each observable (like ∇)

posn: $\langle x \rangle = \int_{-\infty}^{\infty} x P(x) dx = \int_{-\infty}^{\infty} x |\Psi(x)|^2 dx$

PE : $\langle U \rangle = \int_{-\infty}^{\infty} U(x) |\Psi(x)|^2 dx$

$\boxed{\text{not all operators are nice}}$

$|\vec{p}|$ $\langle \vec{p} \rangle = \int_{-\infty}^{\infty} \Psi^*(x) \frac{\hbar}{i} \frac{\partial}{\partial x} \Psi(x) dx$

momentum operator $p = \frac{\hbar}{i} \frac{\partial}{\partial x}$

- we'll stick to simple ones like $\langle x \rangle$

- spread about mean? stats!

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

$\boxed{x_{best} = \langle x \rangle \pm \Delta x}$

$\}$ Can formalize uncertainty! Fourier analysis

) energy comes from time-indep Schrodinger

$$\boxed{\frac{\partial^2 \Psi}{\partial x^2} = -\frac{2m}{\hbar^2}(E-\mathcal{U})\Psi}$$

freepart: $\frac{\partial^2 \Psi}{\partial x^2} = -\left(\frac{2mE}{\hbar^2}\right)\Psi$

- take spatial derivatives once Ψ is known

... energy is the eigenvalues

[like $a = -\omega^2 x$ for oscillator]

) Ψ is continuous, as are its derivatives

Probabilities? like double slit expt

Some rules

(1) if we have a well-defined event (start/end) that can take place alternate ways AND we can't tell which (2 slits @ once)

total Ψ is the sum of all alternates!

$$\Psi_{tot} = \Psi_1 + \Psi_2 + \dots \Psi_n$$

$$P_{event} = |\Psi_1 + \Psi_2 + \dots \Psi_n|^2$$

Constr interference = high event prob
Destr. interference of alternatives = low prob.

Solutions are $\psi = c_1 e^{ikx} + c_2 e^{-ikx}$ $(c_1, c_2 \in \mathbb{C})$

<u>using $\psi(a) = 0$</u>

$$0 = c_1 e^{ika} + c_2 e^{-ika} \Rightarrow \boxed{\frac{c_1}{c_2} = -e^{-2ika}}$$

<u>using $\psi(-a) = 0$</u>

$$\Rightarrow \boxed{\frac{c_1}{c_2} = -e^{2ika}}$$

Combining, $\boxed{c_1 = -c_2}$ & $e^{ika} = e^{-ika} \Rightarrow \boxed{ka = n\pi \quad n \in N_1}$

Since $\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi$ $k^2 = \frac{2mE}{\hbar^2}$

$$\Rightarrow \boxed{E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}}$$ quantized levels

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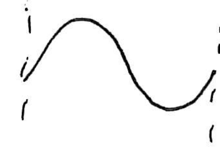
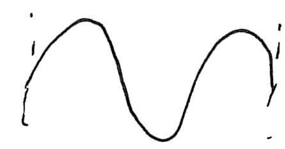
$\psi(x) = c_1 (e^{ikx} - e^{-ikx})$ how about c_1?

<u>unit prob. over all space!</u> "normalize"

$$1 = \int_{-\infty}^{\infty} |\psi|^2 dx \Rightarrow c_1 = \frac{1}{\sqrt{a}}$$

using our form for k, c_1 we have 2 types of solns char. by symmetry

$$\psi^-(x) = \frac{1}{\sqrt{a}} \sin\left(\frac{n\pi x}{a}\right)$$ odd parity 

$$\psi^+(x) = \frac{1}{\sqrt{a}} \cos\left[\frac{(n-\frac{1}{2})\pi x}{a}\right]$$ even parity 

and $E_n^+ = \dfrac{(n-\frac{1}{2})^2 \pi^2 \hbar^2}{2ma^2}$ $\quad E_n^- = \dfrac{n^2 \pi^2 \hbar^2}{2ma^2}$

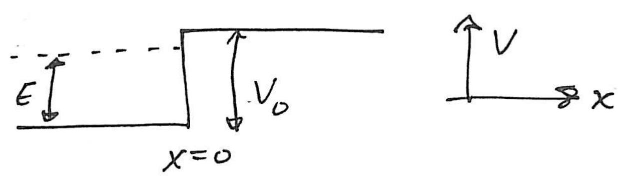
! Lowest energy is not zero, but $E_1^+ = \dfrac{\pi^2 \hbar^2}{8ma^2}$

- zero-point E ... always motion
- more nodes in solution $\Rightarrow$ higher energy ... "harmonics"
- discrete energies

Average posn? $\langle x \rangle = \displaystyle\int_{-\infty}^{\infty} x |\psi|^2 dx = \emptyset$ (from symmetry alone...!)

i.e., middle of well! for any n

$\boxed{\text{Potential step}}$



$$V(x) = \begin{cases} 0 & x<0 \\ V_0 & x>0 \end{cases}$$

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

• V is a function of x only, so is ψ. WHY?

[• Schrodinger eqn is seperable if V is indep of time

$\Psi(x,t) = \psi(x)\,u(t) \Rightarrow$ 2 Schröd eqns $\begin{cases}\text{time-dep}\\ \text{time-indep}\end{cases}$

$u(t) = (\text{const})\, e^{-iEt/\hbar}$]

anyway: $$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - V(x)\right)\psi = 0$$

• like free-particle, but $E \to E - V(x)$

so let $\boxed{k^2 = \frac{2mE}{\hbar^2}}$ as before

also $\boxed{q^2 = \frac{2m(E-V_0)}{\hbar^2}}$

for $x<0$, what is general soln?

w/o step, just freeparticle wave $\longrightarrow$

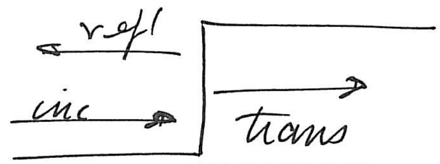
w/step: chance of reflected wave $\longleftarrow$

$$\psi(x) = e^{ikx} + Re^{-ikx}$$

$$\psi(x) = e^{ikx} + Re^{-ikx}$$

- incident wave $\longrightarrow$

reflected wave $\longleftarrow$



$$\boxed{\begin{array}{c} 1 + |R|^2 = |T|^2 \\ \text{conservation} \end{array}}$$

from prob. density

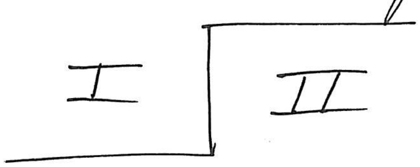
! we miss the transmitted wave (or absorbed)

- like opaque glass $E < V_0$
- $E > V_0$ some transm expt.

with out step: $\psi = e^{ikx}$ same as incident!

<u>reflected</u>: some density backscattered, frac R

<u>transm</u>: what is not reflected passes $x = 0$, frac T



- 2 regions
- in I: two waves - <u>interf</u>
- in II: only 1

So: in I $(x<0)$ $\quad \psi = e^{ikx} + Re^{-ikx}$

in II? particle has $E < V_0$ ... not an "allowed" region

must be decaying soln

formally, $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\underbrace{\left[E - V(x)\right]} = 0$

negative in region II!

in I, have ~ $a = -\omega^2 x$ oscillates $e^{\pm ikx}$

in II, have ~ $a = +\omega^2 x$ decays $e^{\pm \kappa x}$

so $\psi_{II} = T e^{iqx}$

(reject exp incr soln) $\begin{cases} iq = \text{real} \\ q^2 = \frac{2m(E - V_0)}{\hbar^2} < 0 \end{cases}$

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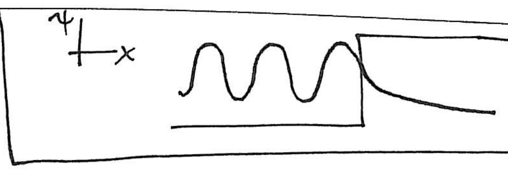
probability conservation



some penetration of barrier!

$$1 - |R|^2 = \frac{q}{k}|T|^2 = \sqrt{\frac{E - V_0}{E}}\,|T|^2$$

$\boxed{\text{at } E = V_0\text{, perfect reflection}}$

wavefunction continuous @ boundary

$$1 + R = T$$

$$\Rightarrow \quad |R|^2 = \left(\frac{k-q}{k+q}\right)^2 \qquad |T|^2 = \frac{k}{q}\cdot\frac{4kq}{(k+q)^2}$$

So what?

interesting aspects:

1) Classical: particle going over a step slows down to conserve E, but is never reflected

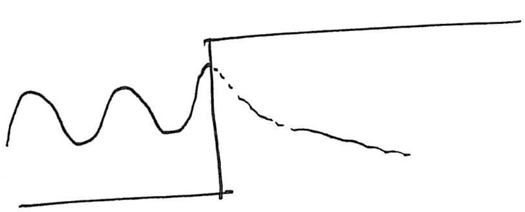
QM: probability that particle is reflected, like light

2) $E \gg V_0$ $(q \to k)$ reflected portion appr. zero

i.e., high energy, step is a small perturbation

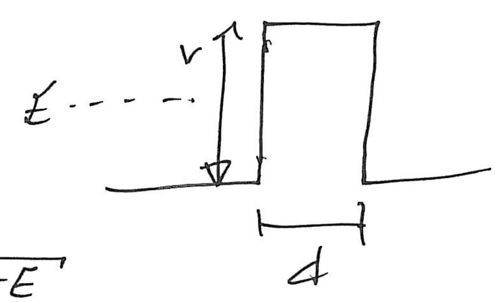
3) $E < V_0$ q is imaginary!

$\psi(x) = T e^{-|q|x}$ exp decay



- particle wave partly penetrates barrier! Classically forbidden

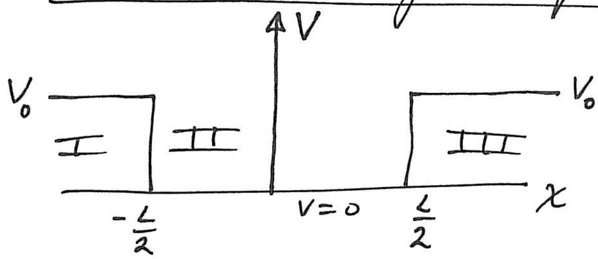
- leads to tunnel effect



$$P_{transit} \sim e^{-d\sqrt{V-E}}$$

particle can jump across!

electron in a finite potential well



- infinite well - bound states
- discrete energy levels

? what if the particle can get out

- if $E > V_0$, much like prior solns
  - scattering occurs, but particle is not trapped

- $E << V_0$ like ∞ well

- how about $E \sim V_0$?

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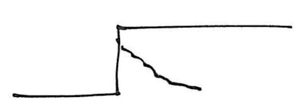
regions I, III solutions to Schrodinger must be decaying

$$\psi_3 = Ce^{-\gamma x} \qquad \psi_1 = \pm Ce^{\gamma x} \qquad \text{where } \gamma^2 = \frac{2m}{\hbar^2}(V_1 - E)$$

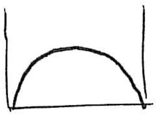


$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi \qquad \text{or} \qquad -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = (E-V)\psi$$

Recall if $E < V$, then $\frac{\partial^2\psi}{\partial x^2} \propto \psi$ decaying

$E > V$, then $\frac{\partial^2\psi}{\partial x^2} \propto -\psi$ oscillating in region II, $V=0$ ... solution is like free-particle solution

$$\psi_2 = A\cos kx \quad \text{or} \quad \psi_2 = A\sin kx \qquad k^2 = \frac{2m}{\hbar^2}E$$

 or  pick <u>cos</u> soln for now

<u>Conditions to match solutions</u>: ψ and $\frac{\partial\psi}{\partial x}$ cont. @ boundaries

$$\Rightarrow \quad \psi_1\left(-\tfrac{L}{2}\right) = \psi_2\left(-\tfrac{L}{2}\right) \qquad \psi_2\left(+\tfrac{L}{2}\right) = \psi_3\left(+\tfrac{L}{2}\right)$$

& similar for $\frac{\partial\psi}{\partial x}$

$$A\cos\left(k\tfrac{L}{2}\right) - Ce^{-\gamma L/2} = 0 \qquad Ak\sin\left(k\tfrac{L}{2}\right) - C\gamma e^{-\gamma L/2} = 0$$

- 2 equations, linear in A & C
- there is a solution iff determinant of coeff vanishes

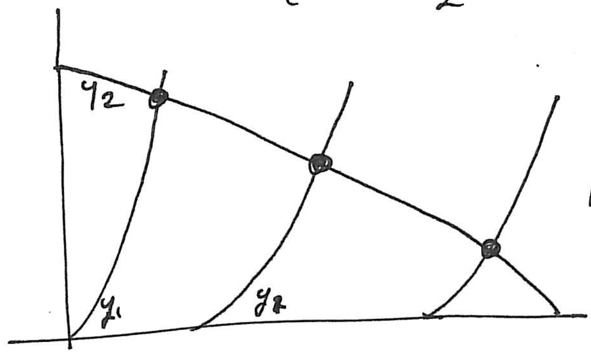
$$\begin{vmatrix} \cos\left(k\frac{L}{2}\right) & -e^{-\gamma L/2} \\ k\sin\left(k\frac{L}{2}\right) & -\gamma e^{-\gamma L/2} \end{vmatrix} = 0$$

$$\Rightarrow \quad k\tan\left(\frac{kL}{2}\right) = \gamma \qquad \text{or} \qquad \sqrt{E}\tan\left(\frac{2mEL^2}{4\hbar^2}\right)^{1/2} = \sqrt{V_1 - E}$$

no analytic soln...

we can solve this graphically

let $m = m_e$ $\quad \frac{L}{2} = 0.5\,\text{nm}$ $\quad V_1 = 1.6\times10^{-18}\,J = 10\,eV$



plot $y_1 = \sqrt{E}\tan\sqrt{\frac{2m}{\hbar^2}E\cdot\frac{L^2}{4}}$

$y_2 = \sqrt{V_1 - E}$

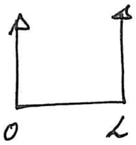
intersections = solutions

- only certain values of E are solns for $E < V_1$
- states are <u>still</u> discrete, quantized
- quantization is no longer simple as in infinite well case

<u>General remarks</u>

- deeper / broader well $\Rightarrow$ more bound states
  like atoms w/ more protons . . .

-

Particle in a box 

$\psi_n = \sqrt{\frac{2}{L}}\,\sin\left(\frac{n\pi x}{L}\right), \quad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$

expected value of x? uncertainty?

$$\langle x\rangle = \int_0^L \psi\, x\, \psi\, dx = \int_0^L \frac{2}{L}\, x \sin^2\left(\frac{n\pi x}{L}\right) dx \qquad u = \frac{n\pi x}{L},\ dx = \frac{L}{n\pi}dx$$

$$= \left(\frac{2}{L}\right)\left(\frac{L}{n\pi}\right)\int_0^{n\pi}\left(\frac{L}{n\pi}\right) u \sin^2 u\, du$$

$$= \left(\frac{2L}{n^2\pi^2}\right)\left[\frac{u^2}{4} - \underbrace{\frac{1}{4}u\sin(2u) - \frac{1}{8}\cos(2u)}_{\text{zero!}}\right]_0^{n\pi}$$

$$= \frac{2L}{n^2\pi^2}\left(\frac{n^2\pi^2}{4}\right) = \boxed{\frac{L}{2} = \langle x\rangle} \quad \text{as expected}$$

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uncertainty? stats! $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$

$$\langle x^2\rangle = \int_0^L \psi\, x^2\, \psi\, dx = \left(\frac{2}{L}\right)\left(\frac{L}{n\pi}\right)\left(\frac{L^2}{n^2\pi^2}\right)\int_0^{n\pi} u^2 \sin^2 u\, du$$

$$= \frac{2L^2}{n^3\pi^3}\left[\frac{u^3}{6} + \underbrace{(3-6u^2)\sin 2u - 6u\cos 2u}_{\text{zero!}}\right]_0^{n\pi}$$

$$= \frac{2L^2}{n^3\pi^3}\left(\frac{n^3\pi^3}{6}\right) = \boxed{L^2/3 = \langle x^2\rangle}$$

$$\Rightarrow \boxed{\Delta x = \sqrt{L^2/3 - L^2/4} = \frac{L}{2\sqrt{3}}}$$

how about Δp? symmetric, equal prob of $\rightarrow$ or $\leftarrow$

$$\Rightarrow \langle p \rangle = 0$$

formally, $\langle p \rangle = \int_{-\infty}^{\infty} \psi^* \frac{\hbar}{i} \frac{\partial}{\partial x} \psi \, dx$

$\langle p^2 \rangle$? we know $p^2 = 2mE$ for a free particle

so $\langle p^2 \rangle = 2mE_n$ (or $\int \psi^* \left(-\hbar^2 \frac{\partial^2}{\partial x^2}\right) \psi \, dx$)

thus $\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{2mE_n} = \frac{n\pi\hbar}{L}$

so $\underline{\Delta x \, \Delta p = \frac{n\pi\hbar}{L} \cdot \frac{L}{2\sqrt{3}} = \frac{n\pi\hbar}{2\sqrt{3}} > \frac{\hbar}{2}}$

uncertainty is satisfied