

From late 19<sup>th</sup>, early 20<sup>th</sup> century:

light: wave and particle (photon)

matter: particle and wave (de Broglie)

so, if matter behaves like a wave, what is the wave function?

ex: periodic travelling water waves:

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

$\Psi$  is the amplitude of the displacement of water at position  $x$ , time  $t$

for a particle, what does  $\Psi(x, t)$  mean?

$\Rightarrow$  this is one of the fundamental things about Quantum Mechanics

current interpretation:

e.g.  $\Psi(x, t)$  for an electron = "amplitude" for finding the electron at  $x, t$

$\Psi$  can be a complex number: has real and imaginary part

## Review of complex numbers

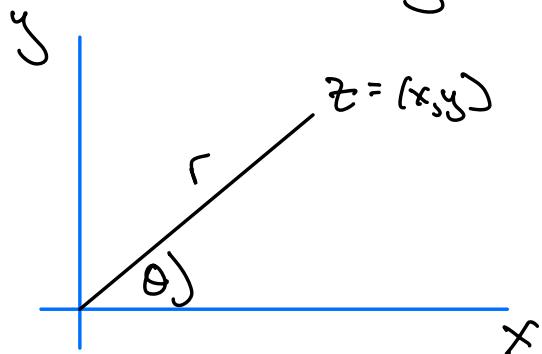
let  $z$  be complex number

let  $i = \sqrt{-1}$  so  $i^2 = -1$

can write  $z = x + iy$

$x$  = "real part of  $z$ " =  $\operatorname{Re}(z)$

$y$  = "imaginary part of  $z$ " =  $\operatorname{Im}(z)$



can write  $x = r \cos \theta$

$$y = r \sin \theta$$

$$\Rightarrow z = r \cos \theta + i r \sin \theta$$

$$= r (\cos \theta + i \sin \theta)$$

$\sin \theta$  &  $\cos \theta$  can be expanded around  $\theta = 0$  using the usual Taylor series:

$$\cos \theta = 1 - \frac{\theta^2}{2} + \frac{\theta^4}{4!} - \dots$$

$$\sin \theta = \theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - \dots$$

$$\text{so } \cos\theta + i\sin\theta = 1 + i\theta - \frac{\theta^2}{2!} - \frac{i\theta^3}{3!} + \frac{\theta^4}{4!} + \frac{i\theta^5}{5!} - \dots$$

now use  $i^2 = -1$

$$\text{so } -\frac{\theta^2}{2!} = + \frac{(i\theta)^2}{2!}$$

$$-i\frac{\theta^3}{3!} = i \cdot i^2 \frac{\theta^3}{3!} = \frac{(i\theta)^3}{3!}$$

$$\frac{\theta^4}{4!} = (i^2)^2 \frac{\theta^4}{4!} = \frac{(i\theta)^4}{4!}$$

and so on

so can write

$$\cos\theta + i\sin\theta = 1 + i\theta + \frac{(i\theta)^2}{2!} + \frac{(i\theta)^3}{3!} + \frac{(i\theta)^4}{4!} + \dots$$

now expand  $e^x$  for small  $x$  using Taylor expansion

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots$$

$$\text{so } \cos\theta + i\sin\theta = e^{i\theta} !$$

$$\text{then can write } z = r e^{i\theta} = x + iy$$

$$\text{where } x = r \cos\theta$$

$$y = r \sin\theta$$

$$r = \sqrt{x^2 + y^2}$$

$$\tan\theta = y/x$$

"complex conjugate" of  $z$  defined as

$$z^* = r e^{-i\theta} = x - iy$$

$$z = r e^{+i\theta} = x + iy$$

$|z|$  is "absolute value" of complex number  $z$   
and  $z = r = \sqrt{x^2 + y^2}$

try  $z \cdot z^* = (x+iy)(x-iy)$

$$= x^2 + iyx - iyx - (iy)^2$$

$$= x^2 + y^2$$

so  $|z| = \sqrt{zz^*} = \sqrt{x^2 + y^2} = \sqrt{\text{Re}(z) + \text{Im}(z)^2}$

complex numbers are very useful for many engineering applications (like AC circuits)

back to QM:

$\Psi(x, t)$  is complex, amplitude for finding a particle at position  $x$ , time  $t$

what does amplitude mean?

current interpretation:

$|\Psi(x, t)|^2$  = probability of finding particle at location  $x$ , time  $t$

but probability is a tricky thing - probability of finding particle exactly at  $x, t$  gets smaller

as you make  $x, t$  more precise

so define probability  $P$  (finding particle between location  $x$  and  $x+dx$ ) is:

$$P(x, x+dx) = |\Psi(x, t)|^2 dx$$

so  $|\Psi(x, t)|^2$  is probability per length  
or "probability density"

$$P(x, x+dx) = \int_x^{x+dx} |\Psi(x, t)|^2 dx$$

which means

$$P(x=-\infty, x=+\infty) = \int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1$$

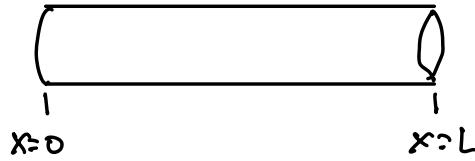
because particle has to be somewhere!

ex: particle is equally likely to be anywhere in a tube of length  $L$

$\Rightarrow$  if particle is equally likely to be at any location in tube, then there is no fine dependence at each location

$$\begin{aligned} \text{so } \Psi(x, t) &= \Psi(x) = C \quad \text{for } 0 \leq x \leq L \\ &= 0 \quad \text{for } x < 0 \text{ or } x > L \end{aligned}$$

where  $C$  is a constant



probability normalization requires:

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \Psi(x,t) dx = \int_{-\infty}^{\infty} |\Psi(x,t)|^2 \Psi(x) dx = 1$$

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = \underbrace{\int_{-\infty}^0 |\Psi(x,t)|^2 dx}_{\Psi=0} + \underbrace{\int_0^L |\Psi(x,t)|^2 dx}_{\Psi=L} + \underbrace{\int_L^{+\infty} |\Psi(x,t)|^2 dx}_{\Psi=0}$$

$$= \int_0^L C^2 dx = C^2 L = 1$$

so  $C = 1/\sqrt{L}$

what is prob to find particle in 1st half of tube?

$$P(0, L) = \int_0^{L/2} |\Psi(x)|^2 dx = \frac{1}{L} \int_0^{L/2} dx = \frac{1}{L} \cdot \frac{L}{2} = \frac{1}{2} \quad \checkmark$$

ex: free particle moving  $w/v = \frac{\omega}{k}$   $\omega = 2\pi f$ ,  $k = \frac{2\pi}{\lambda}$

$$\psi(x, t) = A e^{i(kx - \omega t)} = A \cos(kx - \omega t) + A i \sin(kx - \omega t)$$

this is the most general wave equation for a free particle

what is probability of particle being between  $x_1$  and  $x_2$  locations?

$$\begin{aligned} P(x_1, x_2) &= \int_{x_1}^{x_2} |\psi|^2 dx = \int_{x_1}^{x_2} A e^{i(kx - \omega t)} A e^{-i(kx - \omega t)} dx \\ &= A^2 \int_{x_1}^{x_2} dx = A^2 (x_2 - x_1) = A^2 \Delta x \end{aligned}$$

but shouldn't the particle have a definite location?

QM says: 1. before you measure it, a particle does not have a definite location  
 2. but it can have a definite probability  
 200 4/7  $\Rightarrow$  very revolutionary!

## Properties of particles

ex: what is average position of a particle described by wave function  $\Psi(x, t)$ ?

classical statistics: average age of all students

$$\overline{\text{age}} = \frac{\sum_{i=1}^N \text{age}_i}{N} \quad \frac{\text{sum all ages}}{\#\text{Students}}$$

$$\text{Rewrite: } \overline{\text{age}} = \sum_{i=1}^N \frac{1}{N} * \text{age}_i$$

sum each age weighted by  $\frac{1}{N}$

"weight" is same for all students

can say that weight  $\frac{1}{N}$  is probability for each student:  $P(\text{age}_i) = \frac{1}{N}$

$$\text{so average is } \overline{\text{age}} = \sum_{i=1}^N P(\text{age}_i) \cdot \text{age}_i$$

$$\text{so for any average } x: \overline{x} = \sum x \cdot P(x)$$

in QM we use amplitude  $\Psi(x)$  and write something similar:

$$\overline{x} = \int_{-\infty}^{\infty} \Psi^*(x) \cdot x \cdot \Psi(x) dx$$

400 5/7

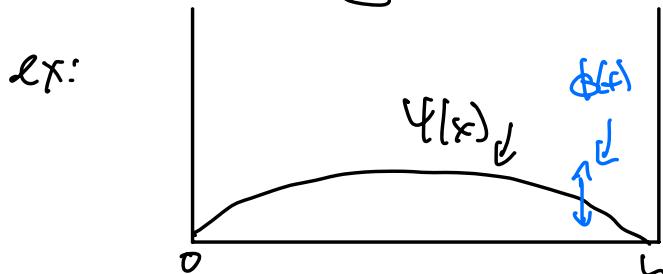
ex: particle is in a box of length  $L$

wave function  $\Psi(x, t)$  is not a travelling wave!

assume:  $\Psi(x, t) = \psi(x) \phi(t)$

$\Rightarrow \psi(x)$  is function of position

$\Rightarrow$  at any  $x$   $\phi(t)$  is how amplitude changes



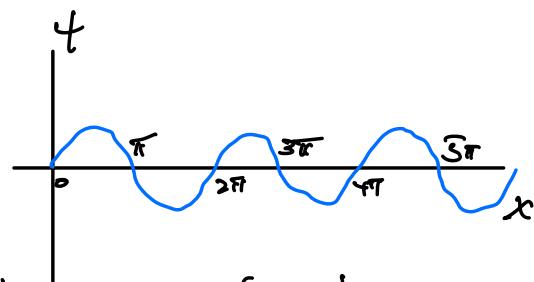
for  $\psi(x)$  try  $\psi(x) = A \sin(kx)$   $0 \leq x \leq L$   
 $= 0$   $x < 0, x > L$  outside boundary

if  $\psi(x=0, x=L) = 0$  then by continuity, want

$\psi(x=0) = \psi(x=L) = 0$  at boundaries

$$\Rightarrow \psi(0) = A \sin(0) = 0 \quad \checkmark$$

$$\psi(L) = A \sin(kL) = 0$$



so  $\psi(L) = 0$  when  $kL = n\pi$   $n=0, 1, 2, \dots$

$$\text{or } k_n = n \cdot \frac{\pi}{L} \quad k_n \text{ is quantized}$$

but then we always get discrete values

of wavelengths when we constrain a wave to have boundaries

e.g. violin, guitar, ...

normalize:  $\int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx = 1$

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^0 |\psi(x)|^2 dx + \int_0^L |\psi(x)|^2 dx + \int_L^{\infty} |\psi(x)|^2 dx$$

$$= \int_0^L |\psi(x)|^2 dx = A^2 \int_0^L \sin^2 kx dx$$

$$= A^2 \int_0^L \frac{1}{2} (1 - \cos 2kx) dx$$

$$= A^2 \left[ \frac{L}{2} - \frac{\sin 2kx}{2k} \right]_0^L$$

$$\sin 2kL = \sin \left( 2 \cdot \frac{n\pi}{L} \cdot L \right) = 0$$

so  $\int_0^L |\psi(x)|^2 dx = \frac{A^2 L}{2} = 1$

means  $A = \sqrt{\frac{2}{L}}$

$$\psi(x) = \sqrt{\frac{2}{L}} \sin(k_n x) \quad k_n = \frac{n\pi}{L} \quad n =$$

$$\text{de Broglie: } p = \frac{h}{\lambda} = \frac{h}{2\pi} \cdot \frac{2\pi}{\lambda} = \hbar k$$

so if  $k$  is quantized so is  $p$ !

$$p_n = \hbar k_n = n \cdot \frac{\hbar \pi}{L} \quad n = 0, 1, 2, \dots$$

consider  $n=0$ : then  $\psi(x) = \sqrt{\frac{2}{L}} \sin(k_0 x) = 0$

but if  $\psi(x)=0$  inside the box, then no particle anywhere!

$\Rightarrow$  this tells you

1.  $v=0$  not allowed
2.  $p_n = n \frac{\hbar \pi}{L}$   $n=1, 2, 3, \dots$  so  $p_0$  does not exist!

$\Rightarrow$  particle can not be sitting still with no velocity

$\Rightarrow$  QM says even if you cool the particle to absolute 0 temp ( $T=0$ ) it has to have a non-zero momentum and therefore a non-zero energy!

non relativistic energy  $E = KE = \frac{p^2}{2m}$

$$\text{so } E_n = \frac{p_n^2}{2m} = \left(n \frac{\hbar \pi}{L}\right)^2 \frac{1}{2m} = n^2 \frac{(\hbar \pi)^2}{2mL}$$

energy is also quantized!

now calculate average position of particle in box

$$\bar{x} = \int_0^L \psi(x)^* x \psi(x) dx \quad \psi(x) = \sqrt{\frac{2}{L}} \sin(k_n x)$$

$$\text{so } \psi \text{ is real so } \psi^* = \psi$$

$$\text{then } \bar{x} = \int_0^L |\psi(x)|^2 x dx = \int_0^L \frac{2}{L} x \sin^2 x dx$$

$$= \frac{2}{L} \left[ \frac{x^2}{4} - x \frac{\sin(2kx)}{4k} - \frac{\cos(2kx)}{8k^2} \right]_0^L$$

$$\sin 2kL = \sin \left( 2 \cdot \frac{n\pi}{L} \cdot L \right) = 0$$

$$\sin(0) = 0$$

$$\cos(2kL) = \cos \left( 2 \cdot \frac{n\pi}{L} \cdot L \right) = \cos(2\pi \cdot n) = 1$$

$$\cos(0) = 1$$

so only  $\frac{L^2}{4}$  term survives

$$\bar{x} = \frac{2}{L} \frac{L^2}{4} = \frac{L}{2} \text{ as expected}$$

but what does "average position" mean?

$\Rightarrow$  averaged over many measurements!

so if you perform many measurements and count  $\ell$  times you measure  $x$  between  $0 - 0.1L$

$$0.1L - 0.2L$$

$$0.2L - 0.3L$$

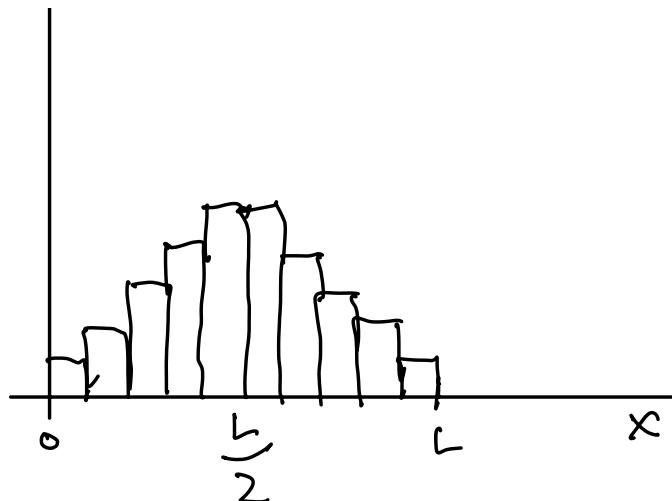
!

$$0.9L - 1.0L$$

this is a "histogram"

plot will show

average at  $\frac{L}{2}$



Wave equation

in  $E \in M$ , for travelling EM wave we have wave equation

$$\frac{\partial^2 E}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2} = 0$$

200 4/9

$E$  is a wave that satisfies that wave equation  
for quantum mechanics:

if  $\Psi(x, t)$  is a wave function, there must be a  
wave equation

for a free particle of mass  $m$ :

$$\Psi(x, t) = A e^{i(kx - \omega t)} = A [\cos(kx - \omega t) + i \sin(kx - \omega t)]$$

with the deBroglie relations

$$p = \frac{h}{\lambda} = \frac{h}{2\pi} \cdot \frac{2\pi}{\lambda} = \hbar k$$

$$E = hf = \frac{h}{2\pi} \cdot 2\pi f = \hbar \omega$$

so can write

$$\underline{\Psi}(x, t) = A e^{i \left( \frac{p}{\hbar} x - \frac{E}{\hbar} t \right)} = A e^{i \left( \frac{p x - E t}{\hbar} \right)}$$

if you take  $\frac{\partial \Psi}{\partial t}$  you get

$$\begin{aligned} \frac{\partial \Psi}{\partial t} &= \frac{\partial}{\partial t} A e^{i \left( \frac{p x - E t}{\hbar} \right)} \\ &= \left( -i \frac{E}{\hbar} \right) A e^{i \left( \frac{p x - E t}{\hbar} \right)} \\ &= -i \frac{E}{\hbar} \Psi \end{aligned}$$

$$\text{so write } i\hbar \frac{\partial \Psi}{\partial t} = i\hbar \left( -i \frac{E}{\hbar} \right) \Psi = E \Psi$$

we can interpret  $i\hbar \frac{\partial}{\partial t}$  as an "operator"  $\hat{E}$

$$\text{where } \hat{E} \Psi = E \Psi$$

$\Psi$   $\uparrow$   
operator energy value

$$\begin{aligned} \text{also try } \frac{\partial \Psi}{\partial x} &= \frac{\partial}{\partial x} A e^{i \left( \frac{p x - E t}{\hbar} \right)} \\ &= i \frac{p}{\hbar} A e^{i \left( \frac{p x - E t}{\hbar} \right)} = i \frac{p \Psi}{\hbar} \end{aligned}$$

$$\text{so momentum operator } \hat{p} = -i\hbar \frac{\partial}{\partial x}$$

$$\text{and } \hat{p}\psi = p\psi$$

think of these operators as "projecting" quantities from wave functions

Quantum theory: can use momentum and energy operators to find average values of momentum & energy

ex: for particle in a box, no time dependence of the box

$$\text{so } \psi(x) = \sum \frac{1}{L} \sin(kx) \quad k = \frac{n\pi}{L} \text{ as above}$$

$$\text{and average } x \text{ is } \bar{x} = \frac{L}{2}$$

what is average momentum?

(AKA "expectation value" of momentum)

$$\bar{p} = \int_0^L \psi^*(x) \hat{p} \psi(x) dx$$

$$= \int_0^L \sum \frac{1}{L} \sin(kx) * -i\hbar \frac{d}{dx} \sum \frac{1}{L} \sin(kx) dx$$

$$= -i\hbar k \int_0^L \sin(kx) \cos(kx) dx = 0$$

because particle spends equal time going in both directions inside box!

what is average energy?

for  $\bar{E}$  use energy operator  $\hat{E} = \frac{\hat{p}^2}{2m} = \frac{1}{2m} \left( -i\hbar \frac{\partial}{\partial x} \right) \left( -i\hbar \frac{\partial}{\partial x} \right)$

$$= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

$$\bar{E} = \int_0^L \psi^* \hat{E} \psi dx$$

$$= \int_0^L \frac{1}{2} \sin(kx) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \sin(kx) \right) dx$$

$$\frac{\partial^2}{\partial x^2} \sin(kx) = k \frac{\partial}{\partial x} \cos(kx) = -k^2 \sin(kx)$$

so  $\bar{E} = \frac{1}{2} \int_0^L \sin^2(kx) \cdot \frac{\hbar^2 k^2}{2m} dx$

$$= \frac{\hbar^2 k^2}{mL} \int_0^L \sin^2(kx) dx$$

$$= \frac{\hbar^2 k^2}{mL} \int_0^L \frac{1 - \cos(2kx)}{2} dx$$

$$= \frac{\hbar^2 k^2}{mL} \cdot \frac{L}{2} = \frac{\hbar^2}{2m} \cdot \left( \frac{n\pi}{L} \right)^2$$

so  $\bar{E}_n = n^2 \frac{\hbar^2 \pi^2}{2mL^2}$  is also quantized

so average energy is just the energy for the particle in the  $n^{\text{th}}$  state

## Schrodinger equation

non-relativistically, we have

$$\bar{E} = KE = \frac{1}{2}mv^2 = \frac{1}{2} \frac{m^2v^2}{m} = \frac{p^2}{2m}$$

$$\text{so } \frac{p^2}{2m} = \bar{E}$$

$$\text{so why not } \frac{p^2}{2m}\bar{\Psi} = \bar{E}\bar{\Psi} \quad (\bar{\Psi}(x,t))$$

now write out the operators:

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

$$\hat{p}^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$$

$$\hat{E} = i\hbar \frac{\partial}{\partial t}$$

turn operator equation into differential equation  
for a free particle:

$$\hat{KE}\Psi = \frac{\hat{p}^2}{2m}\Psi \Rightarrow -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

$$\hat{E}\Psi \Rightarrow i\hbar \frac{\partial \Psi}{\partial t}$$

so energy equation  $\hat{KE}\Psi = \hat{E}\Psi$  gives us

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

what about a particle not free?

e.g. electron in H atom

$\Rightarrow$  not free is because of potential energy!

$\Rightarrow$  PE's almost always do not have any time dependence

let  $U(x)$  be potential energy as a function  
of position

then imagine PE operator  $\hat{P}E = \hat{U}(x)$

classically:  $E = KE + PE$

so extend free particle diff eqn above:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + U(x)\Psi = i\hbar \frac{\partial \Psi}{\partial t} \leftarrow \text{Schrodinger equation}$$

total energy operator  $(\hat{K}E + \hat{U})\Psi$

note: if  $U(x)$  only and not a function of time

$$\text{then } \Psi(x,t) = \Psi(x)e^{-iEt/\hbar} - \Psi(x)e^{-iwt}$$

is a solution because

$$\begin{aligned} i\hbar \frac{\partial \Psi}{\partial t} &= i\hbar \Psi(x) \frac{\partial}{\partial t} e^{-i\omega t} \\ &= i\hbar \Psi(x) (-i\omega) e^{-i\omega t} \\ &= \hbar\omega \Psi(x) e^{-i\omega t} = \hbar\omega \Psi(x, t) \end{aligned}$$

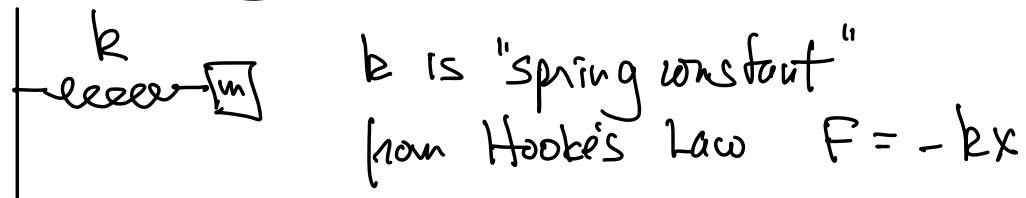
but  $\hbar\omega = E$  from de Broglie

so operator eqn is

$$\hat{K}E \Psi(x, t) + \hat{U}(x) \Psi(x, t) = E \Psi(x, t) \quad \checkmark$$

## Harmonic oscillator

like a spring and mass:



$k$  is "spring constant"  
from Hooke's Law  $F = -kx$

potential energy is  $PE = \frac{1}{2}kx^2$

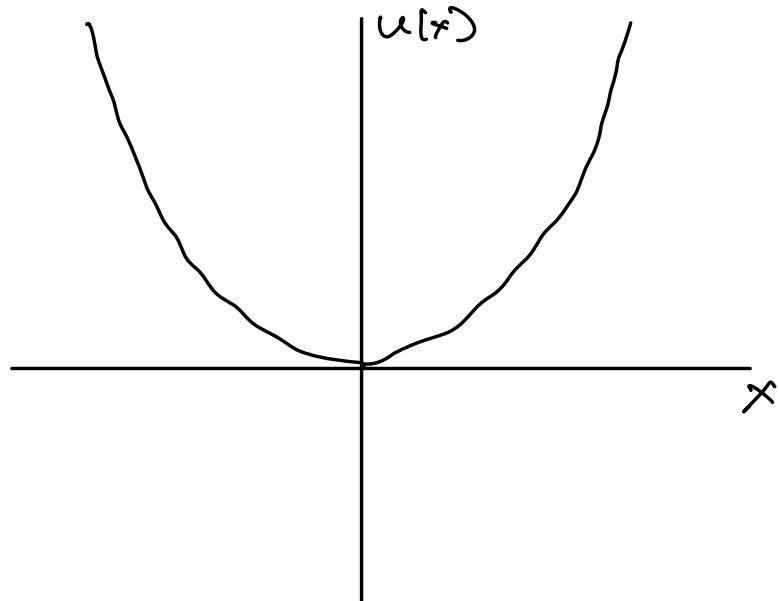
so for QM oscillator  $U(x) = \frac{1}{2}kx^2$

and  $\omega = \sqrt{\frac{k}{m}}$  so  $k = m\omega^2$

$$U(x) = \frac{1}{2}m\omega^2 x^2$$

the potential energy looks like this:

potential



Schrodinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + \frac{1}{2} m \omega^2 x^2 \psi(x) = E \psi(x)$$

this is a difficult differential eqn

answer:  $\psi_n(x) = N_n e^{-\frac{\beta^2 x^2}{2}} H_n(\beta x)$

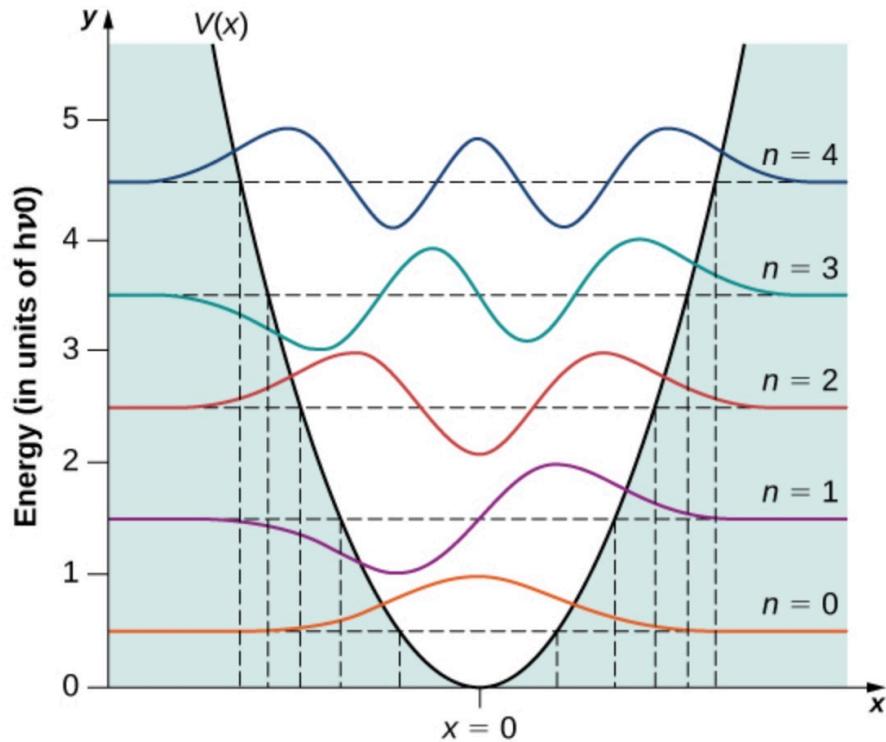
wave function  
for each energy  
level  $n$

normalization  $\int_{-\infty}^{\infty} \psi_n^2(x) dx = 1$

$$N_n = \sqrt{\frac{m\omega}{\pi\hbar^2}}$$

"Hermite  
polynomial"

wave function looks like this:



energy is found to be

$$E_n = \left(n + \frac{1}{2}\right) \hbar \omega \quad n = 0, 1, 2, \dots$$

ground state:  $n=0, E_0 = \frac{1}{2} \hbar \omega$

excited state:  $n=1, E_1 = \frac{3}{2} \hbar \omega$

⋮

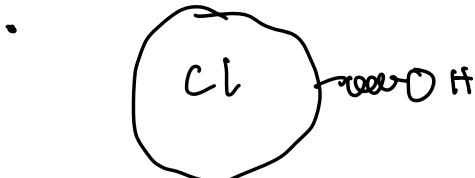
energy levels separated by

$$\Delta E = E_{n+1} - E_n$$

$$= \left(n + 1 + \frac{1}{2}\right) \hbar \omega - \left(n + \frac{1}{2}\right) \hbar \omega = \hbar \omega$$

can use this to model quantised energy levels of molecules like hydrogen chloride HCl

- Cl molecule mass is 35x more than H



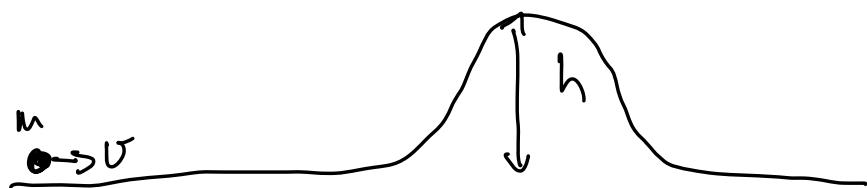
⇒ observed oscillation lowest frequency measured to be  $88.8 \text{ THz}$  ( $\text{THz} > 10^{12} \text{ Hz}$ )

$$\Rightarrow \Delta E = hf = 6.63 \times 10^{-34} \text{ J-s} \times 88.8 \times 10^{12} \frac{1}{\text{s}} \times \frac{1 \text{ eV}}{1.6 \times 10^{-19} \text{ J}} \\ = 0.37 \text{ eV}$$

### Quantum Tunneling

classically:  $E_{\text{tot}} = KE + PE$

ex: ball and hill



$$\text{ball has } KE = \frac{1}{2}mv^2$$

$$PE \text{ at top of hill } PE = mgh$$

- as ball goes up the hill,  $KE$  is converted to  $PE$

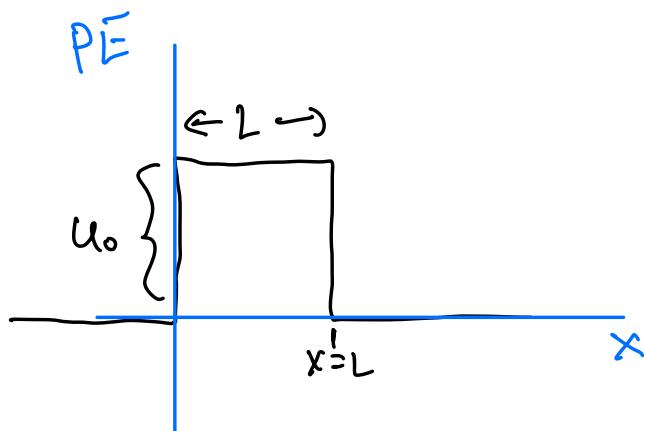
- ball needs  $KE \geq PE$  to get to the top and go over to other side

in quantum world:

$$\text{let } U(x) = 0 \quad x < 0$$

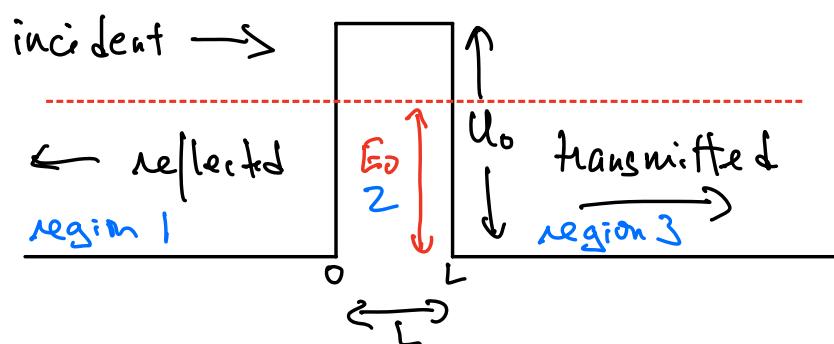
$$U_0 \quad 0 \leq x \leq L \quad U_0 \text{ constant}$$

$$0 \quad x > L$$



$U(x)$  acts like a (energy) potential barrier

⇒ a particle is a wave coming in from  $x = -\infty$  and hits barrier. Particle has energy  $E_0 < U_0$



this situation is described by Schrödinger equation

$\Rightarrow$  suppose situation has no time dependence

$$\Psi(x, t) = \Psi(x)$$

$\Rightarrow$  form equation in each region I, II, III

$$\text{region 1: } -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_1}{\partial x^2} = E_0 \Psi_1 \quad -\infty < x < 0$$

$$\text{region 2: } -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_2}{\partial x^2} + U_0 \Psi_2 = E_0 \Psi_2 \quad 0 \leq x \leq L$$

$$\text{region 3: } -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_3}{\partial x^2} = E_0 \Psi_3 \quad 0 < x < \infty$$

continuity requires  $\Psi_1(0) = \Psi_2(0)$

$$\Psi_2(L) = \Psi_3(L)$$

continuity of derivative requires  $\left. \frac{d\Psi_1}{dx} \right|_0 = \left. \frac{d\Psi_2}{dx} \right|_0$

$$\left. \frac{d\Psi_2}{dx} \right|_L = \left. \frac{d\Psi_3}{dx} \right|_L$$

region 1: no potential so free wave

$\Rightarrow$  incident wave moving to right

$$\text{so } \Psi_{in} = I e^{ikx}$$

amplitude of  $\Psi_{in} = I$

probability of measuring incoming wave

$$\text{is } I^* I, \text{ or } |I|^2$$

$\Rightarrow$  reflected wave moving to left  
 $\therefore \Psi_r = R e^{-ikx}$

amplitude of  $\Psi_r = R$

probability of measuring reflected wave  
is  $R^* R$  or  $|R|^2$

total wave function in region 1:

$$\Psi_1(x) = \Psi_{in}(x) + \Psi_r(x) \\ = I e^{ikx} + R e^{-ikx}$$

region 3: also no potential

and only a transmitted wave

$$\Psi_3(x) = \Psi_t(x) = T e^{ikx}$$

amplitude of  $\Psi_3$  is  $T$

probability of measuring transmitted wave  
is  $T^* T$  or  $|T|^2$

we don't know  $I, R, T$  but if we did then  
we can calculate probability of incident wave  
getting through barrier to be

$$P_{trans} = \frac{|T|^2}{|I|^2} \leftarrow \text{transmission}$$

how can something get through the  
barrier? have to examine region 2!

note: in region 1, 2, 3,  $E_0 = \frac{p^2}{2m}$

use  $p = \hbar k$  to write  $E_0 = \frac{\hbar^2 k^2}{2m}$

$$\text{solve for } k = \frac{2m\sqrt{E}}{\hbar}$$

Region 2: Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_2(x)}{dx^2} + U_0 \psi_2(x) = E_0 \psi_2(x)$$

$$\text{Rewrite: } -\frac{\hbar^2}{2m} \frac{d^2 \psi_2}{dx^2} = \underbrace{(E_0 - U_0)}_{\tilde{E}_0 < U_0} \psi_2(x)$$

$$\tilde{E}_0 < U_0 \text{ so } E_0 - U_0 < 0$$

$$\text{then } \frac{d^2 \psi_2}{dx^2} = -\frac{2m}{\hbar^2} (E_0 - U_0) \psi_2(x)$$

$$= \underbrace{\frac{2m}{\hbar^2} (U_0 - E_0)}_{\text{positive quantity}} \psi_2(x)$$

$$\beta^2 = \frac{2m}{\hbar^2} (U_0 - E_0)$$

$$\text{so } \frac{d^2 \psi_2(x)}{dx^2} = \beta^2 \psi_2(x)$$

general solution is  $\psi_2(x) = A e^{-\beta x} + B e^{\beta x}$

$$\beta = \sqrt{\frac{2m(U_0 - E_0)}{\hbar^2}}$$

as  $U_0 \rightarrow \infty$ , barrier gets higher and  $\beta \rightarrow \infty$   
 so  $e^{-\beta x} \rightarrow 0$

but  $e^{\beta x} \rightarrow \infty$  so  $\beta$  must be very small but non zero!

now apply continuity conditions

continuity of  $\psi$  at boundaries

$$\text{region 1: } \psi_1 = I e^{ikx} + R e^{-ikx}$$

$$2: \psi_2 = A e^{-\beta x} + B e^{\beta x}$$

$$3: \psi_3 = T e^{ikx}$$

$$\text{region 1/2 boundary: } \psi_1(0) = \psi_2(0)$$

$$\text{so } I + R = A + B$$

$$2/3 \quad " \quad \psi_2(L) = \psi_3(L)$$

$$A e^{-\beta L} + B e^{\beta L} = T e^{ikL}$$

continuity of derivatives:

$$\text{region 1/2 boundary: } \left. \frac{d\psi_1}{dx} \right|_0 = \left. \frac{d\psi_2}{dx} \right|_0$$

$$\left. \frac{d\psi_1}{dx} \right|_0 = ik I e^{ikx} \Big|_0 - ik R e^{-ikx} \Big|_0$$

$$= ik I - ik R$$

$$\left. \frac{d\psi_2}{dx} \right|_0 = -\beta A e^{-\beta x} \Big|_0 + \beta B e^{\beta x} \Big|_L$$

$$\text{so } ik(I - R) = -\beta A + \beta B$$

$$\text{Region 2/3 boundary: } \left. \frac{d\psi_2}{dx} \right|_L = \left. \frac{d\psi_3}{dx} \right|_L$$

$$\text{so } -\beta A e^{-\beta L} + \beta B e^{\beta L} = ikT e^{ikL}$$

so we have 4 equations

$$I + R = A + B \quad \text{continuity at } 1/2$$

$$A e^{-\beta L} + B e^{\beta L} = T e^{ikL} \quad " \quad " \quad 2/3$$

$$ik(I - R) = -\beta A + \beta B \quad " \quad \frac{d}{dt} \left. \frac{d\psi}{dx} \right| \text{ at } 1/2$$

$$-\beta A e^{-\beta L} + \beta B e^{\beta L} = ikT e^{ikL} \quad " \quad " \quad " \quad 2/3$$

what we want is the transmission probability

$$P(\text{transmission}) = \frac{T^2}{|I|^2} = \left| \frac{T}{I} \right|^2$$

so take the 4 equations and divide by  $I$  to get

$$1 + \frac{R}{I} = \frac{A}{I} + \frac{B}{I}$$

$$\frac{A}{I} e^{-\beta L} + \frac{B}{I} e^{\beta L} = \frac{T}{I} e^{ikL}$$

$$ik \left( 1 - \frac{R}{I} \right) = -\beta \frac{A}{I} + \beta \frac{B}{I}$$

$$-\beta \frac{A}{I} e^{-\beta L} + \beta \frac{B}{I} e^{\beta L} = ik \frac{T}{I} e^{ikL}$$

4 equations, 4 unknowns:  $\frac{A}{I}, \frac{B}{I}, \frac{R}{I}, \frac{T}{I}$

so far for  $T/I$  after a lot of algebra!

$$\frac{I}{I_0} = \frac{e^{-kL}}{\cosh(\beta L) + i(\frac{\Gamma}{2}) \sinh(\beta L)}$$

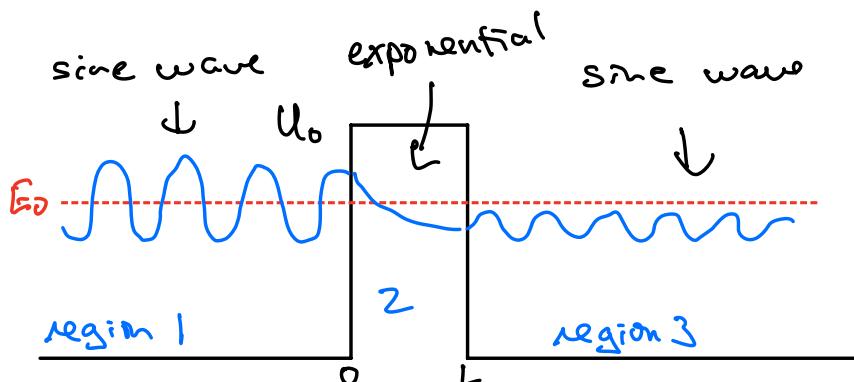
where  $\cosh(\beta L) = \frac{e^{\beta L} + e^{-\beta L}}{2}$  } hyperbolic  
 $\sinh(\beta L) = \frac{e^{\beta L} - e^{-\beta L}}{2}$  functions

$$\gamma = \frac{\beta}{k} - \frac{k}{\beta}$$

then  $P(\text{transmission}) = \left[ \frac{I}{I_0} \right]^2$

$$= \frac{1}{\cosh^2(\beta L) + \left(\frac{\Gamma}{2}\right)^2 \sinh^2(\beta L)}$$

very strong dependence on barrier width  $L$



This is "quantum tunneling" and is basis of solid state transistor technology!