[Not included in Quiz-2]

classmate

Date

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LECTURE - 21

1 QUANTUM MECHANICS

we have a wave function, that depends on the dof of the particle and time.

↳ So for a single particle in 1D, its $\Psi(x,t)$

↳ for a box of N quantum particles in 3D,

$$\Psi(x_1, y_1, z_1, x_2, y_2, z_2, \ldots, x_n, y_n, z_n, t)$$

If you define this Ψ for a system → you can find anything for the system,

Eg in statistical mechanics, if we calculate ~~if we~~ the partition function, then we can calculate everything.

So how do we calculate Ψ, → its given by the Schrödinger's eqn.

So 2 steps → find Ψ for a system
→ All physical observables can be then expressed as operators

mathematical operation

Eg linear momentum
of a 1D system

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

$\sqrt{-1}$

$h/2\pi$ reduced planck's constant.

a simple operator of nature.

Whenever you see a hat/cap above a variable, it means its an operator.

So this $\hbar$ being in a 10^{-34}! It's what takes us from continuous ~~xxx~~ classical to discrete quantum

in all quantum mechanical operators, take $\lim_{\hbar \to 0}$, you get back classical physics.

So now to get the linear momentum of a 1D system at a particular x

- find ψ
- express the value as an operator
- operate the operator on ψ
- you'll get a scalar value times the same wave function

And the scalar value is the magnitude you want of the quantity

this is now the mathematics of quantum mechanics has been built.

So we have to define these operators.

Eg $\hat{K} = \frac{\hat{P}\hat{P}}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

kinetic energy operator

hence apply $\hat{P}$ twice

for 1D case, replace $\hat{P}_x$

whichever $\hat{P}$ you're using

once on ψ

you'll get scalar $\times\ \psi$

then apply $\hat{P}$ on that again.

eg $\hat{P}_x \Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial x}$

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

scalar measure of linear momentum

2 SCHRÖDINGER'S EQUATION

its used to get Ψ
It tells us how Ψ evolves with times and with your dof.

So we had the hamiltonian

convert it to an operator

$H = K + U$

$\Rightarrow \hat{H} = \hat{K} + \hat{U}$

So the ~~hamilto~~ schrodingers eqn gives:

$\hat{H}\Psi(x,t) = E\Psi(x,t)$

scalar, called total energy.

so, for 1D, it'll become :

$$-\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + \hat{U}(x)\,\Psi(x,t) = E\,\Psi(x,t)$$

Potential energy operator it'll be a simple scalar function → it'll come in the examples.

→ This is called the time independent schrödinger equation

time independent because it doesn't have $\frac{\partial \Psi}{\partial t}$ or such terms,

it does not tell you how Ψ evolves with time. All that it tells you is at a given time, how Ψ evolves with x.

[we'll later do a schrödinger eqn in which we'll have $\frac{\partial \Psi}{\partial t}$, how Ψ evolves with time] so then, we talked of a couple of systems

3. PARTICLE CONFINED IN A 1-D BOX

so a wire with length >> diameter

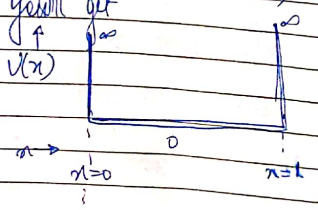
so its 1D

and we have insulators on either side, so the electrical potential looks like :

$$V(x) = 0 \qquad 0 < x < l$$
$$V(x) = \infty \quad , x = 0, l.$$

Assume potential of the wire is 0, and under electrostatic conditions, it's same everywhere.

so on your potential curve, you'll get



so now we solved the schrödinger eq^n last class to get

$$\psi_n(x) = \sqrt{\frac{2}{l}} \sin\left(\frac{n\pi x}{l}\right)$$

and

$\psi_n^*(x)\ \psi_n(x)$ gives the probability density

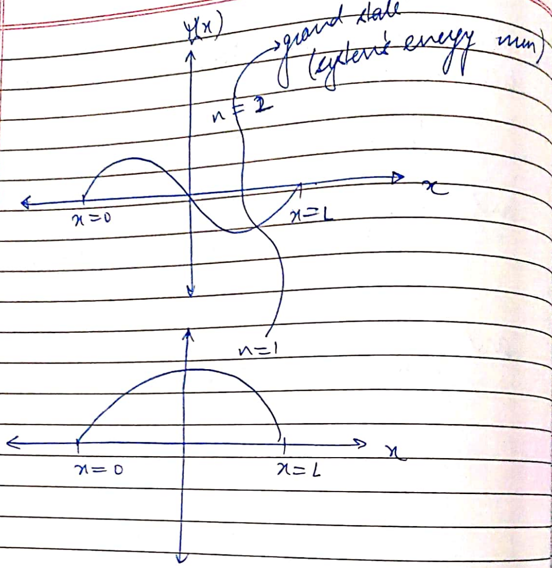
and $$\langle x \rangle = \int_{x_1}^{x_2} x P(x)\, dx$$

$$= \int_{x_1}^{x_2} x\ \psi^*(x)\ \psi(x)\, dx$$

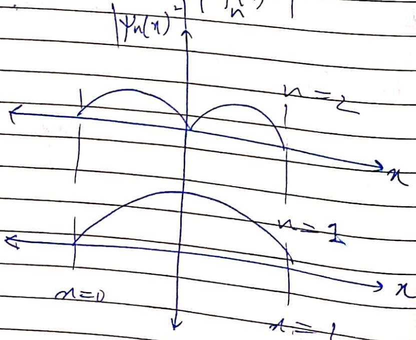
and then we can graph the probability

NOTE: In QM, $\frac{h^2}{8ml^2}$ is the fundamental unit of energy

3.

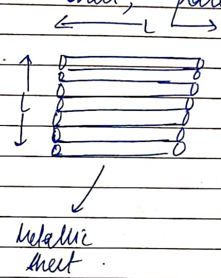


And for probability density, we can use $|\psi_n(x)\, \psi_n^*(x)|$ which is $|\psi_n(x)^2|$

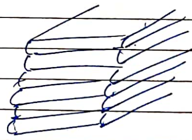


4. EXTENSION OF 1D BOX MODEL.

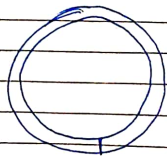
① To build a metallic sheet, place multiple wires



② Make a 3D box using such sheets.



③ Take the ~~circular~~ wire and wrap it into a circle



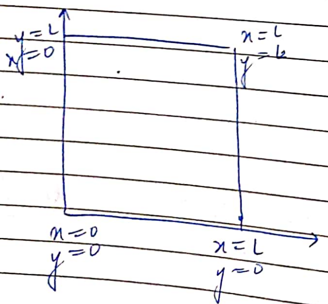
This is a very simple ~~system~~ model of an atom → a nucleus in the and e^- around.

(4) Earlier, we had infinite potential barriers on either sides,

now, we can have finite barriers on either sides by placing some other metal instead of insulators

metal-2 | metal-1 | metal-2

C. PARTICLE IN A 2D BOX



$V(x,y) = 0 \quad , \quad 0 < x < L$
$\qquad\qquad\qquad\quad 0 < y < L$

$V(x,y) = \infty$, outside.

So, inside the sheet potential is 0

↓

potential energy is 0.

So we write the schrödinger eqⁿ :

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]\Psi(x,y) = E\,\Psi(x,y)$$

Now, we'll separate $\Psi(x,y) = X(x)\,Y(y)$

[separate characters

we do this because we know ψ will be like this because ψ is related to probability and ∵ x and y are uncoupled/independent, the probability can be separated.

$$Y(y)\left(\frac{-\hbar^2}{2m}\frac{\partial^2 X(x)}{\partial x^2}\right)$$

$$+\ X(x)\left(\frac{-\hbar^2}{2m}\frac{\partial^2 Y(y)}{\partial y^2}\right)$$

$$= E\ X(x)\ Y(y)$$

separate into E_1 and E_2

for first part

for 2nd part

$\div\ X(x)Y(y)$ on both sides

$$\frac{1}{X(x)}\left(\frac{-\hbar^2}{2m}\frac{\partial^2 X(x)}{\partial x^2}\right) = E_1$$

$$\frac{1}{Y(y)}\left(\frac{-\hbar^2}{2m}\frac{\partial^2 Y(y)}{\partial y^2}\right) = E_2$$

so we can solve to get

$$E_1 = \frac{n_1^2 h^2}{8mL^2} \qquad E_2 = \frac{n_2^2 h^2}{8mL^2}.$$

$$E = E_1 + E_2 = \frac{(n_1^2+n_2^2)h^2}{8mL^2}$$

2 quantum No.s.

so you'll get

$$\Psi_{n_1,n_2}(x,y) = \frac{2}{L}\sin\left(\frac{n_1\pi x}{L}\right)\sin\left(\frac{n_2\pi y}{L}\right)$$

ground state: $n_1 = n_2 = 1$ ← that's when energy ~~[illegible]~~ is the least.

and its energy,

$$E_{1,1} = \frac{2h^2}{8mL^2} = \frac{h^2}{4mL^2}$$

first excited state,

$$E_{1,2} = \frac{5h^2}{8mL^2}$$

$$E_{2,1} = 5h^2/8mL^2$$

so these states, $n_1 = 2$ $n_2 = 1$
and $n_1 = 1$ $n_2 = 2$

are different states, ∵ the ψ for these 2 states is different
↳ so they are different states.
But they have the same energy
↳ they are called degenerate states
and degeneracy is 2
No. of degenerate states with a given energy value