1st January 2024

⊛ Syllabus on WeLearn.

→ What necessitated a departure from classical physics.
→ Postulates / Axioms of QMech.
→ Schroedinger equation
→ Operators
→ Wave functions
→ eigenvalues
→ Commutation relation.
→ Particle in a potential well (Square well, Scattering, tunelling)
→ Simple Harmonic oscillator (SHO)
(raising and lowering operators approach)
→ Probabilities and expectation values.
→ Heisenberg uncertainty principle.
→ Schroedinger equation in 3D
→ Hydrogen atom, angular momentum.

Reference: Griffiths, Sakurai (lol)

⊛ Evaluation – (a) Internal : 30%

Class Test → 20
(Notice given ahead)
(Best 2/3)

Assignments → Not graded
(every wednesday submission)

Attendance → counted if situation arises.

Class performance → 10 ensured if exam performance is good.

(b) Midsem : 20%

(c) Endsem : 50%

O What is Classical Physics?

The usual answers.

○ What is Classical Physics?

The usual answers.

→ Follows NLM, is macroscopic, EM-theory dictated, etc.

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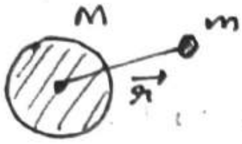
3rd Jan 2024

○ What is Classical physics?

→ Isaac Newton (1687)

→ Law of motion

→ Law of gravitation.

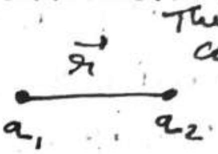


$$\boxed{m\frac{d^2\vec{r}}{dt^2} = \vec{F} = -\frac{GMm}{r^2}\hat{r}}$$

→ Charles Coulomb (1785) Static force? If there is accel there is motion. There is a conundrum.

→ Law of electrostatic force

$$\vec{F} = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r^2}\hat{r}$$



→ Ampere (1823)

→ Faraday (1831)

→ Gauss (1835)

→ Maxwell (1862)

~~Gt~~ Laws of Electrodynamics

i) $\vec{\nabla}\cdot\vec{E} = \frac{\rho}{\varepsilon_0}$

ii) $\vec{\nabla}\cdot\vec{B} = 0$

iii) $\vec{\nabla}\times\vec{E} = -\frac{\partial\vec{B}}{\partial t}$

iv) $\vec{\nabla}\times\vec{B} = \mu_0\left(\vec{J} + \varepsilon_0\frac{\partial\vec{E}}{\partial t}\right)$

→ Lorentz (1895)

→ Laws of electromagnetic force

$$\vec{F} = q(\vec{E} + \vec{v}\times\vec{B})$$

Summary:

Law of motion → $\boxed{m\frac{d^2\vec{r}}{dt^2} = \vec{F}}$

Electromagnetic force diff **Gravitational force**

$\vec{F} = q(\vec{E} + \vec{v}\times\vec{B})$ $\qquad$ $\vec{F} = m\vec{g}$, $\vec{g} = -\frac{GM\hat{r}}{r^2}$

In the static limit,

$\vec{F} = q\vec{E}$ ← Look Similar

- Why is speed of light an universal constant.
- Why is there no velocity dep term here for gravitation? — something like a magnetic component.

Albert Einstein

(STR) $\qquad$ (GTR)

This is all of Classical physics

Ex: Consider a motion under a constant force: (in 1D)

$$m\frac{d^2x}{dt^2} = F = \text{const}.$$

Integrating,

$$\frac{dx}{dt} = u_0 + \int\left(\frac{F}{m}\right)dt = u_0 + \left(\frac{F}{m}\right)t$$

Integrating again,

$$x = x_0 + u_0\int dt + \left(\frac{F}{m}\right)\int t\,dt$$

$$\Rightarrow x = x_0 + u_0 t + \frac{1}{2}\left(\frac{F}{m}\right)t^2$$

x_0, u_0 → const. of integration.

(NLM is silent about these — we given / provide input)

physically, x_0 → Initial position

u_0 → Initial velocity.

Knowing these, the entire future of the particle is determined with certainty. → Classical physics is deterministic

5th Jan 2024

Recall: Classical Physics

↳ Deterministic predictions.

(*) Inbuilt in all theories in classical physics.

(*) 3 Key failures of Classical physics
(Led the ~~the~~ birth of QM)

→ (1) Black body radiation (Max Planck 1900 AD)

→ (2) Photoelectric effect (Albert Einstein, 1905)

→ (3) Spectral lines in photo-emission (Niels Bohr, ~~1930~~ 1913)

All three are connected by light.

What is light?

In vacuum, $\vec{J}=0$, $\rho=0$

then, Maxwell equations become simpler —

(1) $\vec{\nabla}\cdot\vec{E}=0$ (2) $\vec{\nabla}\times\vec{E}=-\frac{\partial\vec{B}}{\partial t}$

(3) $\vec{\nabla}\cdot\vec{B}=0$ (4) $\vec{\nabla}\times\vec{B}=\mu_0\epsilon_0\frac{\partial\vec{E}}{\partial t}$

Usual derivation (as waves) —

$$\vec{\nabla}\times(\vec{\nabla}\times\vec{E}) = \vec{\nabla}\times\left(\frac{-\partial\vec{B}}{\partial t}\right)$$

$$\Rightarrow \vec{\nabla}\times(\vec{\nabla}\times\vec{E}) = \frac{-\partial}{\partial t}(\vec{\nabla}\times\vec{B})$$

$$\Rightarrow \vec{\nabla}\times(\vec{\nabla}\times\vec{E}) = -\frac{\partial}{\partial t}\left(\mu_0\epsilon_0\frac{\partial\vec{E}}{\partial t}\right)$$

$$\Rightarrow \vec{\nabla}(\vec{\nabla}\cdot\vec{E})-\vec{\nabla}^2\vec{E} = -\frac{\partial}{\partial t}\left(\mu_0\epsilon_0\frac{\partial\vec{E}}{\partial t}\right)$$

$$\Rightarrow \boxed{\nabla^2\vec{E}=\mu_0\epsilon_0\frac{\partial^2\vec{E}}{\partial t^2}}$$

(wave equation)

(*) Assignment: Similarly we can show $\nabla^2\vec{B}=\mu_0\epsilon_0\frac{\partial^2\vec{B}}{\partial t^2}$

$\boxed{A1/Q1}$

This is a Kind of propagating solution.

Both electric field and magnetic field satisfy wave equation of the form,

$$\boxed{\nabla^2 f = \frac{1}{v^2}\frac{\partial^2 f}{\partial t^2}}$$

$v \rightarrow$ Speed of propagation of wave.

Speed of electromagnetic wave :

$$v = \frac{1}{\sqrt{\mu_0 \epsilon_0}}$$

$\epsilon_0 \rightarrow$ Permittivity of vacuum (Value Known from Coulomb's Law)

$\mu_0 \rightarrow$ Permeability of vacuum (Value Known from Biot-Savart law)

Pluggin in the values,

$$v \simeq 3 \times 10^8 \ m \cdot s^{-1}$$

(*) Speed of light (say c) :
as measured through astronomical observation first by Ole Roemer in 1676 AD

(*) Maxwell (1864) : 'perhaps light is an electromagnetic wave'

as $\boxed{v \simeq c}$

(1) Black body radiation :

→ Every physical body spontaneously emits electromag radiation

Ex : Heated iron rod, Human body.

→ Such radiation depends on the temperature T of the body.

(*) Wilhelm ~~Wien~~ Wien (1896) :

Spectral density energy : (Energy density of radiation having frequency ν to $\nu + d\nu$

$$u_\nu = \frac{8\pi h}{c^3}\nu^3 e^{-h\nu/K_B T}$$

$K_B \rightarrow$ Boltzmann constant

$h \rightarrow$ A constant needed to make $\frac{h\nu}{K_B T}$ dimensionless.

$\rightarrow$ It describes observations accurately for high frequency (short wave length)

$$\boxed{h\nu >> K_B T}$$

It does not work for low frequency, i.e,

$$h\nu << K_B T$$

(*) Rayleigh - Jeans law: (1900)

$$\boxed{u_\nu = \frac{8\pi K_B T}{c^3}\nu^2}$$

Based on classical consideration.

$\rightarrow$ It works for low frequency, i.e,

$$h\nu << K_B T$$

But fails for,

$$h\nu >> K_B T$$

(*) UV catastrophe

☐ Max Planck guessed the formula as an interpolation b/w these two. Guess the formula.

8th January 2023

○ Recall:

Blackbody radiation —

Wien's Law (1896)

Spectral energy density

$$u_\nu = \frac{8\pi h}{c^3} \nu^3 e^{-h\nu/k_BT}$$

(works for $h\nu >> k_BT$).

Rayleigh-Jeans Law (1900)

$$u_\nu = \frac{8\pi (k_BT)}{c^3} \nu^2$$

(Works for $h\nu << k_BT$)

Blows up as $\nu \to \infty$ (UV catastrophy)

Same year as the RJ formula,

○ Max Planck (1900):

→ Empirical formula — He did not know then how it worked. It only fits the experiment.

→ Matches Wien's formula at $h\nu >> k_BT$, and RJ at $h\nu << k_BT$.

$$\boxed{u_\nu = \frac{8\pi h \nu^3}{c^3} \cdot \frac{1}{e^{h\nu/k_BT} - 1}}$$

⊛ High frequency → $h\nu >> k_BT \Rightarrow e^{h\nu/k_BT} - 1 \approx e^{h\nu/k_BT}$

Thus it becomes Wien's formula,

$$u_\nu = \frac{8\pi h \nu^3}{c^3} e^{-h\nu/k_BT}$$

(But a power of ν is off?).

⊛ Low frequency → $h\nu << k_BT \Rightarrow e^x \approx 1 + x$

$$\Rightarrow e^{h\nu/k_BT} \approx 1 + \frac{h\nu}{k_BT}$$

Thus, it becomes, $u_\nu = \frac{8\pi (k_BT)}{c^3} \nu^2$

(*) In 1901, Planck proposed the notion of <u>hypothetical oscillator</u> to describe black body radiation of frequency ν and having energy as <u>integer</u> multiples of $h\nu$

→ The idea of 'quanta' as a 'mathematical device' that leads to a single formula and 'need not really exist somewhere in nature'

This was a hand-wavy mathematical derivation.

(*) <u>In Summary</u> →

Planck proposed that the energy of a monochromatic beam of radiation with frequency ν should be of the form

$$E = \underbrace{N}_{\text{Integer} \geq 0} \underbrace{h}_{\substack{\text{Constant} \\ \text{(Planck constant)}}} \nu$$

ν → freq of monochromatic radiation.

Also,

$$E = N \underbrace{\left(\frac{h}{2\pi}\right)}_{\hbar} \underbrace{(2\pi\nu)}_{\text{Angular freq}}$$

$$\Rightarrow E = N\hbar(2\pi\nu) = N\hbar\omega$$

(*) We will redefine h as $\hbar$ as convention, generally.

(*) <u>Energy flux</u>: $S = nh\nu$

Energy flux → 'Spectral' form

n → Number of light quanta passing through per unit area, per unit time

But we ~~alway~~ already have the expression for the poynting vector – from Maxwell's electrodynamics

(*) Maxwell's electrodynamics –

$$\nabla^2 \vec{E} = \mu_0 \epsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2} \quad , \quad \nabla^2 \vec{B} = \mu_0 \epsilon_0 \frac{\partial^2 \vec{B}}{\partial t^2}$$

Solutions that describe a monochromatic light beam with frequency ν along z direction.

The solutions of this are,

$$\boxed{\begin{aligned} \vec{E} &= E_0 \cos(kz - \omega t)\,\hat{i} \\ \vec{B} &= \underbrace{B_0}_{E_0/c} \cos(kz - \omega t)\,\hat{j} \end{aligned}}$$

→ Reason why ω is easier to use in $\hbar$ notation.

Energy flux given by Maxwell →

$$\vec{S} = \frac{1}{\mu_0}(\vec{E} \times \vec{B}) = \frac{E_0^2}{\mu_0} \cos^2(kz - \omega t)\,\hat{k}$$

The one we should ~~average~~ compare with Planck's new formula is the time averaged version of this.

Max Planck

$$\boxed{S = n\hbar\nu}$$

Time average of flux:

$$\langle \vec{S} \rangle = \frac{E_0^2}{2\mu_0 c} = \frac{\epsilon_0 E_0^2 c}{2}$$

→ No freq dependence

It says that the flux depends on amplitude, not the frequency as Planck's formula suggests.

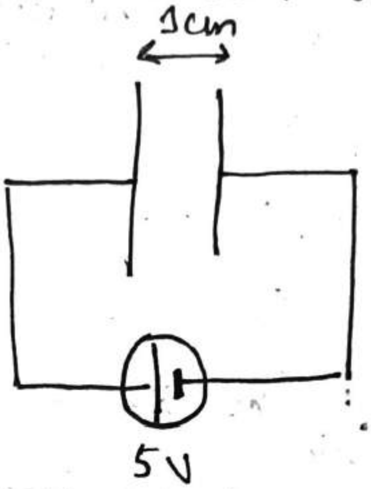
So there is a problem.

There is a Conceptual problem with classical physics.

Now we calculate value of 'n' — To see why there is a problem in certain domains and no problem in others.

Ex 1 : Compute the electric field between two parallel plates that are separated by 1 cm and connected to a 5 V battery.

Soln : Assume that the electric field is uniform.



$$V = \int \vec{E} \cdot d\vec{l} = EL \Rightarrow E = \frac{V}{L}$$

$$\therefore \boxed{E = \frac{5V}{1\,cm} = 500\,V/m}$$

E2

Q1/A2 Compute the peak electric field due to a light beam generated by a 5 watt LED bulb (assume 1 conversion factor — no heat loss) and passing through a square of side 10 cm

E3

Q2/A2 In the two configurations (of E1 and E2), which one has a stronger peak of electric field.

10th January 2024

$\boxed{E4}$ If the LED ~~ligh~~ bulb emits red light with frequency 650 nm in $\boxed{E2}$ then as per planck's proposal, how many light quanta pass through the ~~bulb bulb~~ square persecond.

Soln: $\lambda = 650\text{nm}$ / $A = (10\text{cm})^2$

$W = 5W$, $\boxed{S = nh\nu}$

$$nA = \frac{SA}{h\nu} = \frac{SA\lambda}{hc}$$

$$\Rightarrow nA = \frac{(SA)\lambda}{hc} \Rightarrow nA = \frac{W\lambda}{hc}$$

$$\Rightarrow nA = \frac{(5)(650\times10^{-9})}{(6.626\times10^{-34})(3\times10^{8})}$$

$$= \frac{(5)(650)}{(6.626)(3)} \times 10^{17}$$

$$= 1.6\times10^{19}\ s^{-1}$$

(*) $\boxed{E5}$ (Q3/A2) Estimate the peak electric field caused by a single light-quanta in the $\boxed{E2}$

We will see that Maxwell equation predict correctly in its own domain. But Planck's hypothesis expands it.

(2) Photoelectric effect:

If a light beam falls on a material then electrons are emitted from the material.

(*) Lennard (1902 AD): Observed that the Kinetic energy of the emitted electrons increases if the frequency of incident light beam is increased.

→ This is in conflict with Maxwell equations, as it states that energy of EM wave depends only on the intensity. (not on frequency)

Albert Einstein: (1905)

→ Using Planck's idea of light quanta, the maximum kinetic energy of an emitted electrons ~~should be~~ are given.

$$KE_{max} = h\nu - W$$

Max KE of electron

Energy of light quanta

Bonding energy of the electron (work function)

→ This matched with <u>experiment</u>.

E6 In a photo-electric expt. the max K·E of an emitted electron found to be 0.86 eV and 0.37 eV when corresponding incident lights were violet (400nm) and blue (475nm). Determine the value of the Planck's constant. Does the material show any photoelectric effect if one uses red light beam (620nm)

<u>Soln</u>:

$$0.86 = h(400\times10^{-9}) \cancel{+} W$$

$$0.37 = h(475\times10^{-9}) - W$$

$$\Rightarrow W = h(475\times10^{-9}) \cancel{a} - 0.37$$

$$\Rightarrow$$

$$\cancel{\therefore 0.86 = h(400\times10^{-9}) - h(475}$$

$$\Rightarrow 0.37 - 0.86 = h(75\times10^{-9})$$

$$\Rightarrow h = \frac{(0.37-0.86)(1.6\times10^{-19})}{(75\times10^{-9})} \cancel{J}$$

$$\Rightarrow \boxed{h = 4.14\times10^{-15}\ \cancel{Js}\ eV\cdot s}$$

$$\therefore \cancel{0.37 =}\ W = (4.14)(10^{-15})(475\times10^{-9}) + 0.37$$

$$\Rightarrow \boxed{W = 2.24\ eV}$$

The energy of light quanta of red color = 2.0 eV which is lower than the work function.

③ <u>Spectral lines in photo-emission</u> →

→ Observations

↳ one see only certain lines (wavelengths) that are present in any photo emission spectrum.

④ classically, it should have all ~~the~~ lines.

The energy of light quanta of red color = 2.0 eV
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③ <u>Spectral lines in photo-emission</u> →

→ Observations
↳ one see only certain lines (wavelengths) that are present in any photo emission spectrum.
⊛ classically, it should have all ~~the~~ lines.

<u>12th January 2024</u>

<u>Recall :</u>
⊛ Spectral lines in photo-emission :
Observations : → ~~Only~~ certain wavelengths λ are present in any photo-emission spectrum.

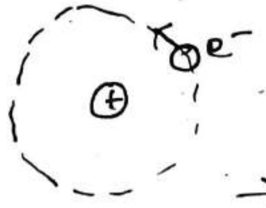
⊛ <u>Johannes Rydberg</u> (1888) :
Visible (to human eyes) spectral lines from hydrogen gas can be expressed as,

$$\boxed{\frac{1}{\lambda} = R_H \left(\frac{1}{2^2} - \frac{1}{n^2} \right)}$$

$n = 3, 4, 5$
R_H → Rydberg constant

⊛ <u>Rutherford (1911) :</u>
From ~~sea~~ <u>scattering</u> experiments
↳ An atom consists of concentrated +ve charge at the centre, surrounded by -vely charged electrons.

<u>Eg :</u> Hydrogen atom →



This is what was hypothesized.
→ A particle in a circular orbit is an accelerating particle
→ <u>Maxwell :</u> An accelerating charged particle will continuous radiate EM waves
So it will radiate energy and fall into proton. (matter of minutes)

⊛ Classical physics →

Force balance :

$$\boxed{\frac{m_e v^2}{r} = \frac{1}{4\pi\varepsilon_0} \cdot \frac{e^2}{r^2}}$$

So we can calculate energy of the electron →

$$\boxed{E = \frac{1}{2} m_e v^2 - \frac{1}{4\pi\varepsilon_0} \cdot \frac{e^2}{r}}$$

Eliminating using the force balance equation,

$$E = \frac{1}{2}\left(\frac{1}{4\pi\varepsilon_0} \frac{e^2}{r}\right) - \frac{1}{4\pi\varepsilon_0} \frac{e^2}{r}$$

$$\Rightarrow \boxed{E = -\frac{1}{2} \frac{e^2}{4\pi\varepsilon_0} \left(\frac{1}{r}\right)}$$

Classical bound state formula

(Total energy is half of potential)

As r is continuous, the electron could be anywhere.

Classically, the electron's orbit can have any r.

⇒ Any energy.

Then how do we explain only certain spectral lines?

This suggests that emitted light can have any wavelength. → NOT consistent with expt.

Maxwell : An atom is not stable!

Niels Bohr (1913):

Somehow electrons stay only on those orbits where angular momentum is quantized.

$$\boxed{m_e v r = n\hbar} \quad , \hbar = \frac{h}{2\pi} \quad , n = 1, 2, 3, 4, \ldots$$

- You can backcalculate from this to get Rydberg formula.

from previous formula,

$$m_e^2 v^2 r^2 = \frac{m_e}{4\pi\varepsilon_0} e^2 r = n^2 \hbar^2$$

- How did he arrive at angular momenta as the thing that is quantized? ① Planck ($E = h\nu$) ② Total Energy

You can start with Rydberg and arrive at Bohr hypothesis ☒ Try

$$\Rightarrow \boxed{\frac{1}{r} = \frac{m_e}{n^2\hbar^2} \frac{e^2}{4\pi\varepsilon_0}}$$

$$\Rightarrow E_n = \frac{-m_e}{2\hbar^2} \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{1}{n^2}$$

(*) Now if an electron jumps from $n = 3, 4, 5, \ldots$ to $n = 2$ energy levels..

Energy of light quanta,

$$\boxed{h\nu = E_n - E_2} \qquad \boxed{\nu = \frac{c}{\lambda}}$$

$$\Rightarrow \frac{1}{\lambda} = R_H \left[\frac{1}{2^2} - \frac{1}{n^2}\right]$$

Where, $\boxed{R_H = \frac{1}{\hbar c} \left(\frac{m_e}{2\hbar^2}\right)\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2}$

⊛ E_7 (A3/Q1)

An experimental physicist finds the wavelength of an EM wave from Hydrogen gas to be ~~100~~ 1010 nm. With a spectrometer having accuracy of 1%. Using Bohr model, determine the initial and final energy levels of the ~~electron~~ corresponding electron. (given $E_1 = -13.6\,eV$)

⊛ Key lessons from Planck, Einstein and Bohr →

1. Energy of the electromagnetic waves are quantized
2. An electron absorbs energy in quanta
3. An electron emits energy in quanta.

The problem lies in the determinism in classical physics

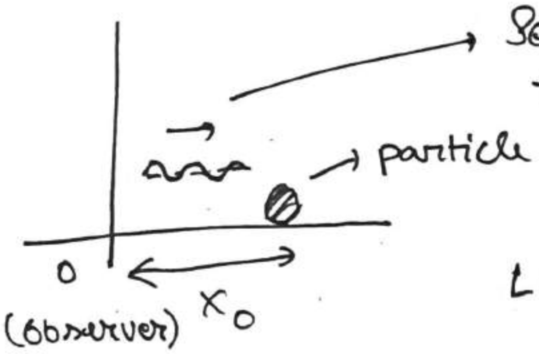
Under const force: $x = x_0 + u_0 t + \frac{1}{2}\left(\frac{F}{m}\right)t^2$
provided we supply x_0 and u_0.

⊛ Is it possible to determine x_0 and u_0 ~~if~~ for any particle, even in principle?

→ All classical laws are 2nd order diff eqns, so two constants of integration. — are they possible to supply.

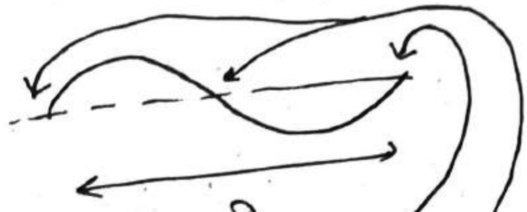
We start with the determinism question. 15th Jan 2024

→ How do we measure the position (say x_0) of a particle?



→ Send photon to particle & count time it takes to come back, and calculate position

But there is a ~~p~~ problem –
Light has <u>finite extent</u>



When it reflects, there must be a <u>node</u>?

~~Δx~~ $\Delta x \sim \frac{\lambda}{2}$ (Node can be)

→ Send a light, measure the delay in arrival time, say t_0, of the reflected wave,

$$\boxed{x_0 = \frac{ct_0}{2}}$$

→ There is an inherent error $\boxed{\Delta x \sim \frac{\lambda}{2}}$

→ We should use smaller λ ~~for~~ for measuring position. (to minimise the error)

(*) How do we measure v_0?

→ Measure the position again, say x_0' after an interval at say t_0'

⇒ $$\boxed{v_0 = \frac{x_0' - x_0}{\frac{(t_0' - t)}{2}}}$$

photon has momentum $= \frac{h}{\lambda}$

But since photon <u>comes back</u>, the particle whose position is being measured <u>gets momentum</u>.

→ In order to reflect the photon the particle's original momentum ($p_0 = mv_0$) changes!

→ Inherent error in momentum measurement

$$\frac{h}{\lambda_3} + p_1 = -\frac{h}{\lambda} + p_2$$

$$\Rightarrow \boxed{\Delta p \sim \frac{2h}{\lambda}}$$

→ To minimize Δp, we should use larger λ

So, Δx and Δp counter each other.

* We note, $\boxed{\Delta x \Delta p \sim h}$

(First primitive form of the <u>Heisenberg Uncertainty Principle</u>)

⇒ $\Delta x\, \Delta p$ is <u>independent of measurement</u>

* We will come back to this.

* Determinism in classical mechanics depends on the condition that cannot be provided.

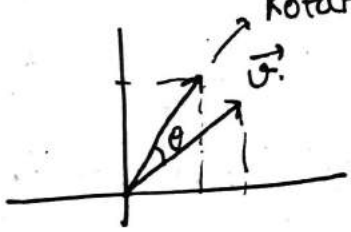
→ x and p are <u>not good variables</u> to describe the quanta.

* <u>Vector Calculus</u> →

An element of a set, known as <u>linear vector space</u>, is called <u>a vector</u>

$v \in V$.

Rotation,



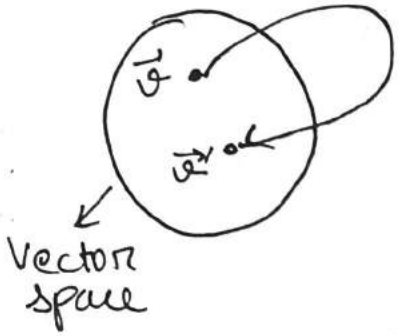
$$v_x' = v_x \cos\theta + v_y \sin\theta$$

$$v_y' = -v_x \sin\theta + v_y \cos\theta$$

Written in matrix form,

$$\begin{pmatrix} v_x \\ v_y \end{pmatrix}' = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} v_x \\ v_y \end{pmatrix}$$

$$\Rightarrow \vec{v}\,' = R(\theta)\,\vec{v}$$



$R(\theta) \longrightarrow \boxed{R(\theta) : V \to V}$

Operator: $\hat{O}$ is a map a linear vector space to itself i.e,
$v' = \hat{O}\, v$ such that $\forall\, v, v' \in V$

(*) Linear: The addition operation is linear.

Here, $R(\theta)$, rotation by ~~ang~~ angle θ is an example of an operator.

(*) Consider operator $\hat{O} = R(\theta = \pi)$

$$v = R_{\theta=\pi}\, v = -v$$

$$\Rightarrow \boxed{R_{\theta=\pi}\, v = \lambda v}\ , \quad \lambda = -1$$

An operator equation of the form,

$$\boxed{\hat{O}\,\psi = \lambda\,\psi}$$

is called an eigenvalue equation, where the vector ψ is called an eigen vector and the complex number λ (in general) is called the eigenvalue.

17th January 2024

We begin by recalling ~~eo~~ eigenvalue equation.

(*) Maxwell's wave equation:

$$\boxed{\nabla^2 \psi = \frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2}} \qquad \psi \to \vec{E}, \vec{B}$$
$$\psi = \psi(t, \vec{x})$$

Which has the solution of the form,

$$\psi = \psi(t, \vec{x}') = \psi_0 e^{i(\vec{k}\cdot\vec{x} - \omega t)}$$

(general form).

An EM wave with angular frequency ω is represented by a complex valued function,

$$\psi = \psi(t, \vec{x}')$$

further, this wave-function ψ also describes a quanta of energy $E = h\nu = \hbar\omega$

Schrodinger ~~of~~ tried to formulate a new way to read off the energy of a wave by combining the eigenvalue method and Planck's hypothesis.

He said that we probably are not reading the physics properly.

Consider the action,

$$\boxed{\begin{aligned} i\hbar \frac{\partial \psi}{\partial t} &= (i\hbar)(-i\omega)\psi \\ &= \hbar\omega\psi \\ &= E\psi \\ &= \hat{H}\psi \end{aligned}}$$

This is an eigenvalue equation where eigenvalue is the energy of the light quanta. (*)

Therefore the operator $\boxed{\hat{O} = i\hbar\frac{\partial}{\partial t}}$

represents the energy operator, or usually called the Hamiltonian operator, $\hat{H}$ (say)

$$\Rightarrow \boxed{i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi}$$

$\boxed{P_x = -i\hbar \frac{\partial}{\partial x}}$ → Momentum operator (You can guess it)

$$\Rightarrow \boxed{\hat{\vec{p}} = -i\hbar \vec{\nabla}}$$

~~As~~ (As $p = \frac{h}{\lambda} = \frac{h}{2\pi} \cdot \frac{2\pi}{\lambda} = \hbar K$)

Nothing is new here, but we invert the question and use this to derive physics (???)

(*) ~~Energy~~ model of Bohr →

Energy of an electron

$$E = \frac{p^2}{2m} + V$$

Hamiltonian operator corresponding to the electron,

$$\boxed{\hat{H} = \frac{\hat{\vec{p}}^{\,2}}{2m} + \hat{V} = -\frac{\hbar^2}{2m}\nabla^2 + V}$$

Like quanta of light, electron should also be described by some wave function Ψ. Such that

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$$

Let us say that this came to us in a dream –

(*) Schrodinger's Equation →

$$\boxed{i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar}{2m}\nabla^2 + V\right)\Psi = \hat{H}\Psi}$$

PDEs are not easy to solve in general.

(*) We will employ a trick to ~~con~~ convert this to two ODEs.

(*) Method of separation of variables:

Ansatz: $\Psi(\vec{x},t) = T(t)\,\psi(\vec{x})$.

Schrödinger equation in (1+1) dimensions →

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

Plugging in the ansatz,

$$\Rightarrow \frac{1}{T(t)}\, i\hbar \frac{\partial T(t)}{\partial t} = \frac{1}{\psi(x)}\left[-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x)\right]$$

$$= E = \text{const}$$

As LHS is func of t, and RHS is func of x.

$$\boxed{i\hbar \frac{dT}{dt} = ET}$$ Time dependant part

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

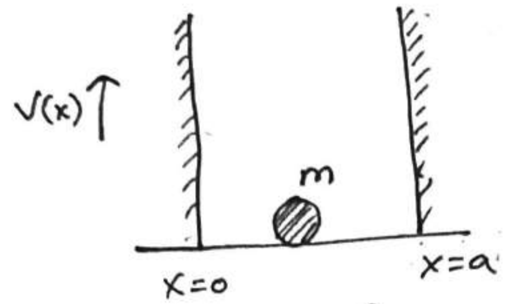
Time independent part.

(*) We start with particle in a box in the next class.

19th January 2024

⊛ Infinite square well → (1+1 D)

Suppose potential $V(x)$ is given as $V(x) = \begin{cases} 0, & 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases}$.



(i) The particle is free inside the box
↳ No force acting on it.

$$\boxed{F = -\frac{\partial V}{\partial x} = 0} \quad \text{for } \cancel{0 \le x \le a} \; 0 < x < a$$

(ii) What about the force at the boundary?

$$F(a_+) = -\lim_{h \to 0^+} \frac{V(a+h) - V(a)}{h}$$
$$= -\infty$$

$$F(a_-) = -\lim_{h \to 0} \frac{V(a-h) - V(a)}{h} = 0$$

The particle experiences an infinite force if it tries to move to the right at $x=a$

At $x=0$, opposite situation arises.

(iii) Within the wall: Total ~~ene~~ energy of the particle,

$$E = \frac{1}{2}mv^2 + V^{\nearrow 0} = \frac{p^2}{2m} \geq 0$$

either 0 or positive

$E=0$ is called the minimum energy configuration. (Ground state)

Now we solve it using <u>Quantum Mechanics</u> →

Schrodinger equation (Time independent)

$$\hat{H}\,\Psi(x) = \frac{\hat{P}^2}{2m}\Psi(x) = E\,\Psi(x)$$

Again, this is an <u>operator</u>.

$$\hat{P} = -i\hbar\frac{d}{dx}$$

$$\Rightarrow \boxed{\hat{H}\,\Psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(\psi(x)\right) = E\,\Psi(x)}$$

2^{nd} order ODE

$$\Rightarrow \frac{d^2\psi}{dx^2} + K^2\psi = 0 \quad , \text{where } K^2 = \frac{2mE}{K^2}$$

<u>Ansatz</u>: $\Psi(x) = e^{mx}$

$$\Rightarrow m^2 + K^2 = 0 \Rightarrow m = \pm iK$$

(Auxilliary eqn)

<u>General Solution</u>: $\boxed{\Psi(x) = Ae^{iKx} + Be^{-iKx}}$

How do we determine the constants A and B?

(In Newtonian case, it was intuitive as x_0 and $\dot{x}_0$)

Time independent Schroedinger equation –

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \psi(x)V(x) = E\,\psi(x) \quad \text{—} \ (1)$$

It is a law of nature and it should remain well defined for all physically plausible domain (i.e, $-\infty < x < \infty$) and for all physically plausible potential (i.e $V(x) < \infty$) → physically plausible

(Think of $V(x) = \infty$ as a limit to infty, not infty)

(*) Well-defined means that the values involved are finite.

Integrating (1), over a small interval around $x = a$

$$\int_{a-\epsilon}^{a+\epsilon} \frac{d}{dx}\left(\frac{d\psi}{dx}\right)dx = \int_{a-\epsilon}^{a+\epsilon} (V - E)\,\psi(x)\,dx$$

why? It must not blow up

as $\epsilon \to 0$

$$\Rightarrow \left.\frac{d\psi}{dx}\right|_{x=a+\epsilon} - \left.\frac{d\psi}{dx}\right|_{x=a-\epsilon} = L < \infty \text{ (finite)} \quad \text{(say)}$$

Now, $$\left.\frac{d\psi}{dx}\right|_{x=a+\epsilon} = \frac{\psi(a+\epsilon) - \psi(a)}{\epsilon}$$

So, $$\Rightarrow \left.\psi(x)\right|_{x=a+\epsilon} - \left.\psi(x)\right|_{x=a-\epsilon} = L\epsilon$$

$$= 0 \quad (\text{as } \epsilon \to 0)$$

$$\Rightarrow \boxed{\psi(a+\epsilon) = \psi(a-\epsilon)}$$

$\psi(x)$ is continuous at $x = a$ (???)

(A) If $V(x)$ is continuous,

$\Rightarrow \psi'(x)$ is also continuous.

(B) If $\boxed{V(x) = V_0\,\delta(x-a)}$

$\psi'(x)$ has a finite discontinuity at $x = a$

(C) $V \to \infty$

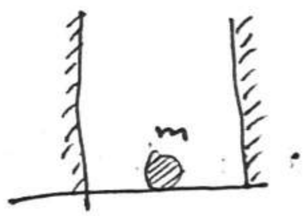
$$\int_{a-\epsilon}^{a+\epsilon} V\,\psi(x)\,dx < L$$

$\to \infty$ (What??)

$$\Rightarrow \psi(a) \int_{a}^{a+\epsilon} V(x)\,dx < L$$

22nd January 2024

Recall: Infinite square well:



$$V(x) = \begin{cases} 0, & 0 \leq x \leq a \\ \infty, & \text{otherwise} \end{cases}$$

Time independent Schroedinger equation:

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

The equation is well behaved if we use well behaved potentials.

General solution: $\boxed{\psi(x) = Ae^{iKx} + Be^{-iKx}}$

$$K^2 = \frac{2mE}{\hbar^2}$$

If $V(x)$ blows up, $\psi(x)$ must go to zero.

We now need to fix the constants A and B.

$\psi(x = 0^-) = 0$ (particle cannot be there - potential is infinity)

$\Rightarrow \boxed{A + B = 0} \Rightarrow \boxed{B = -A}$

Similarly,

$$\psi(x = a^+) = 0$$

$\Rightarrow Ae^{iKa} - Ae^{-iKa} = 0$ → Does not allow us to fix A.

We impose a condition,

$$e^{i2Ka} = 1 = e^{i2n\pi} \Rightarrow Ka = n\pi$$

$$n = 1, 2, 3, \ldots$$

$\therefore E = \frac{\hbar^2 K^2}{2m} = \boxed{\frac{\hbar n^2\pi^2}{2ma^2} = E_n}$ Energy eigenvalues that are allowed

Now, the n^{th} wave function,

$$\Psi_n(x) = Ae^{i\frac{n\pi x}{a}} - Ae^{-i\frac{n\pi x}{a}}$$

$$\Rightarrow \boxed{\Psi_n(x) = D\sin\left(\frac{n\pi x}{a}\right)} \rightarrow \text{Energy eigenfunc/ eigenstate.}$$

We can verify,

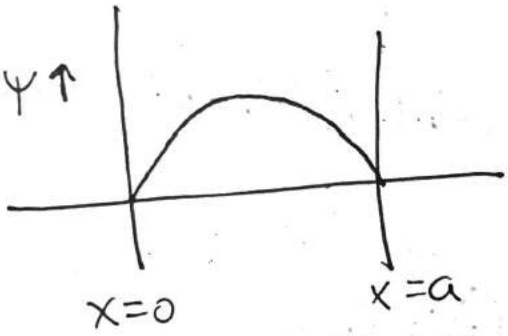
$$\boxed{\hat{H}\Psi_n = E_n\Psi_n} \rightarrow \text{Eigenvalue equation.}$$

now,

$n=1$: $E_1 = \frac{\hbar^2\pi^2}{2ma^2}$ → Noground state.

(minimumenergy configuration)

$\Psi_1 = D\sin\left(\frac{\pi x}{a}\right)$

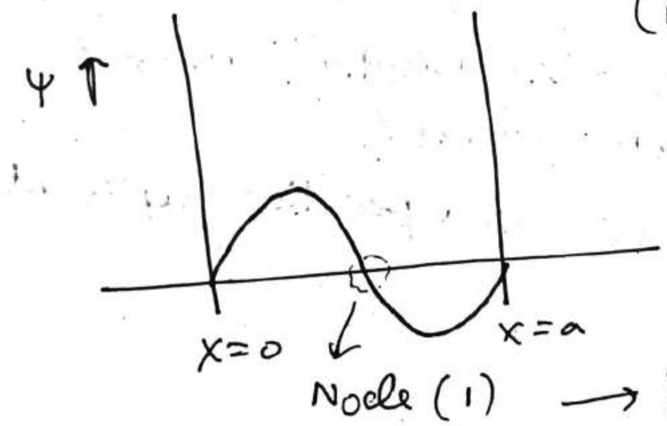


Quantum mechanical ground state.

If $\Delta p = 0$, uncertainty wouldbe violated.

$n=2$: $\boxed{E_2 = \frac{4\pi^2\hbar^2}{2ma^2}} \rightarrow \boxed{\Psi_2 = D\sin\left(\frac{2\pi x}{a}\right)}$

(Firstexcited state)



Node (1) → Exactlyone node.

State canbe determined by counting non-boundary nodes.

(*) Time-dependant part of the Schroedinger eqn $\longrightarrow$

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

We have solved $\psi(x)$,

$$\boxed{\hat{H}\,\psi_n(x) = E_n\,\psi_n(x)}$$

Now,

$$i\hbar \frac{dT(t)}{dt} = E_n T(t)$$

Solution is,

$$\boxed{T = T_0 e^{-i\frac{E_n t}{\hbar}}}$$

Therefore, the full solution to the Schroedinger equation,

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H}\,\psi(x,t)$$

$$\boxed{\Psi_n(x,t) = \psi_0\, e^{-i\frac{E_n t}{\hbar}} \sin\left(\frac{n\pi x}{a}\right)}$$

We have a non-trivial solution (non-zero)

(*) Is this a wave, or not?

Does $\Psi_n(x,t)$ for a particle represent any wave?

Now, put $\frac{E}{\hbar} = \omega$, $n\pi = kx$

$$\Psi = \Psi_0 e^{-i\omega t} \left(\frac{e^{ikx} - e^{ikx}}{2i} \right)$$ → sin x using euler's identity.

$$\Rightarrow \boxed{\Psi(x,t) = \underbrace{C_1 e^{i(kx - \omega t)}}_{\text{wave moving to the right}} + \underbrace{C_2 e^{i(kx + \omega t)}}_{\text{wave moving to the left.}}}$$

(*) What does the wave function Ψ represent for a particle? (open question)

Maxwell's equations —

$$\vec{\nabla} \cdot \vec{E} = \frac{\rho}{\varepsilon_0}, \quad \vec{\nabla} \times \vec{B} = \mu_0 \left(\vec{J} + \varepsilon_0 \frac{\partial \vec{E}}{\partial t} \right)$$

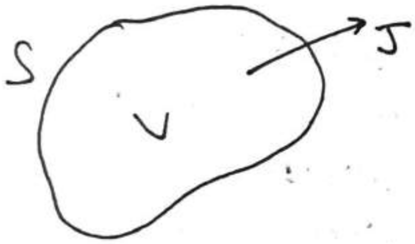
$\rho = \rho(x,t)$ → charge density

$\vec{J} = \vec{J}(x,t)$ → current vector..

Now, we use the identity $\vec{\nabla} \cdot (\vec{\nabla} \times \vec{A}) = 0$

$$\vec{\nabla} \cdot (\vec{\nabla} \times \vec{B}) = 0 = \vec{\nabla} \cdot \vec{J} + \varepsilon_0 \vec{\nabla} \cdot \left(\frac{\partial \vec{E}}{\partial t} \right)$$

$$\Rightarrow \boxed{\vec{\nabla} \cdot \vec{J} + \frac{\partial \rho}{\partial t} = 0}$$ → Charge conservation equation.



$$\frac{d}{dt} \int_V d^3x \, \rho(x,t) = -\int_V d^3x \, (\vec{\nabla} \cdot \vec{J})$$

$$Q \qquad = -\int_S \vec{J} \cdot d\vec{S}$$

→ If no charge is leaking through the surface S, $\int_S \vec{J} \cdot d\vec{S} = 0$, then total charge Q is conserved as $\boxed{\frac{dQ}{dt} = 0}$

The SE also admits situations like this.

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \quad -①$$

$\psi \rightarrow$ complex valued function.

So we can write a conjugate equation,

<u>Conjugate:</u>

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V(x)\,\psi^* \quad -②$$

(Assume V real)

$\psi^* \times ① - \psi \times ② \Rightarrow$

$$i\hbar\left(\psi^*\frac{\partial \psi}{\partial t} + \psi\frac{\partial \psi^*}{\partial t}\right) = -\frac{\hbar^2}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right)$$

$$\Rightarrow \frac{\partial}{\partial t}(\psi^*\psi) = -\vec{\nabla}\left[\frac{\hbar}{2mi}\left(\psi^*\vec{\nabla}\cdot\psi - \psi\vec{\nabla}\cdot\psi^*\right)\right]$$

So analogously,

$$\rho = \psi^*\psi, \quad \vec{J} = \frac{\hbar}{2mi}\left(\psi^*\vec{\nabla}\cdot\psi - \psi\vec{\nabla}\cdot\psi^*\right)$$

$$\rightarrow \boxed{\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0}$$ $\rightarrow$ Conservation equation implied by Schroedinger eqn

$\rightarrow \int d^3x\, \psi^*\psi \rightarrow$ is a conserved quantity

if $\int_S \vec{J}\cdot d\vec{S} = 0$

⊛ At boundary if ψ is zero, then $\vec{J} = 0$.

24th January 2024

Schroedinger eqn $i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$

admits a conservation equation,

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0$$

where $\rho = \psi^*\psi$

$$\vec{J} = \frac{\hbar}{2mi}\left[\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right]$$

If $\int_V d^3x\,(\vec{\nabla}\cdot\vec{J}) = \int_S \vec{J}\cdot d\vec{s} = 0$ (for eg ψ vanishes at boundary)

then $\int d^3x\,\psi^*\psi$ is conserved.

⊛ Max Born (1926) → (Most accepted interpretation)

He gave a statistical interpretation.

$\rho = \psi^*(x,t)\,\psi(x,t)$ is the probability density of finding the particle at point x

⊛ Convention (as in statistics):

Normalization ⇒ Total probability = 1

In QM: Convention is to ~~no~~ normalize wave function as,

$$\int d^3x\,\psi^*\psi = 1$$

→ dimension 3+1

⊛ $\boxed{\text{Q1/A4}}$: Show that for the infinite square well potential (as being studied in class), the normalized energy eigenstates can be expressed as $\psi_1 = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)$ (do it for time independent)

⊛ A will be fixed from this. — the normalization fixes it.

⊛ Consider two solutions (say) Ψ_1 and Ψ_2 such that both satisfy Schroedinger equation:
s.t

$$\boxed{i\hbar \frac{\partial \Psi_1}{\partial t} = \hat{H}\Psi_1} \text{ and } \boxed{i\hbar \frac{\partial \Psi_2}{\partial t} = \hat{H}\Psi_2}$$

are both true.

<u>Claim</u>: Any arbitrary linear combination of Ψ_1 and Ψ_2 ~~are~~ is also a solution of the Schroedinger equation.

<u>Proof</u>: Consider $\Psi_3 = c_1\Psi_1 + c_2\Psi_2$

c_1 and c_2 are two complex numbers.

<u>LHS</u> →

$$i\hbar \frac{\partial \Psi_3}{\partial t}$$

$$= c_1 i\hbar \frac{\partial \Psi_1}{\partial t} + c_2 i\hbar \frac{\partial \Psi_2}{\partial t}$$

$$= c_1 \hat{H}\Psi_1 + c_2 \hat{H}\Psi_2$$

$$= \hat{H}(c_1\Psi_1 + c_2\Psi_2)$$

$$= \hat{H}\Psi_3 \quad \text{(RHS)}$$

→ This result is known as the principle of linear superposition.

⇒ All solutions of the Schroedinger solution forms a linear vector space

⊛ <u>Define</u>: Inner product or dot product on this vector space as,

$$(\Psi, \Psi) = \langle \Psi | \Psi \rangle = \int d^3x \, \Psi^* \Psi$$

$\boxed{E1}$ Compute the inner product between the two following energy eigenstates.

$$\psi_1 = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$$

$$\psi_2 = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right)$$

Soln: $(\psi_1, \psi_2) \equiv \psi_1 \cdot \psi_2 = \langle \psi_1 | \psi_2 \rangle$

$$= \int_0^a \psi_1 \cdot \psi_2 \, dx$$

$$= \int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) dx$$

$$= 0$$

. They are orthogonal to each other. (w.r.t their given linear product)

(*) For different eigenvalues, the eigenstates are orthogonal.

(*) $\boxed{A4/Q2}$: Show that all energy eigenstates form an orthonormal set of vectors, i.e. $(\psi_m, \psi_n) = \delta_{m,n}$

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

(*) If a linear vector space say V along with an inner product $\langle \cdot | \cdot \rangle$ is such that for all vectors ψ,

$$\langle \psi | \psi \rangle < \infty$$

i.e, $(\psi, \psi) \equiv \langle \psi | \psi \rangle = \int d^3x \, \psi^* \psi < \infty$

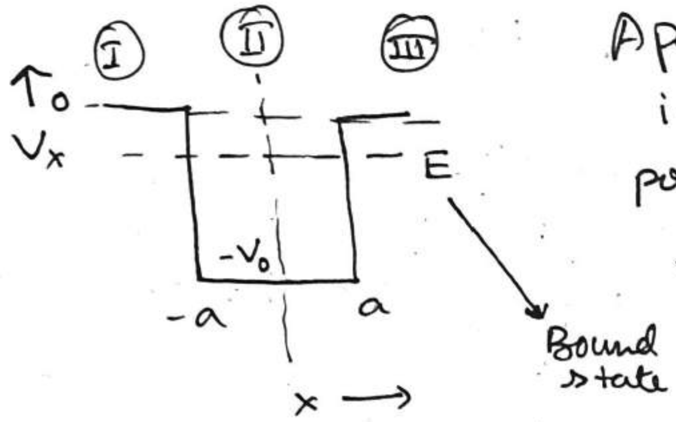
i.e, squared norm is $\|\psi^2\| = (\psi, \psi)$ is finite.

i.e, ψ is square integrable

Then such vector space is called a Hilbert Space.

29th January 2024

Finite Square well →



A particle of mass m is moving in a potential $V(x)$ as

$$V(x) = \begin{cases} -V_0, & |x| \leq a \\ 0, & |x| > a \end{cases}$$

(I) : $x < -a$: $V(x) = 0$

Time - independent Schrodinger equation →

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$E < 0$ (bound state)

$$\Rightarrow \frac{d^2\psi}{dx^2} - \kappa^2\psi = 0 \quad , \quad \kappa^2 = \frac{-2mE}{\hbar^2}$$

General solution : (Ansatz, $\psi \sim e^{\kappa x}$)

$$\psi_I(x) = A_1 e^{\kappa x} + A_2 e^{-\kappa x}$$

Similarly for region (III) : $x > a$:

General solution :

$$\psi_{III} = C_1 e^{\kappa x} + C_2 e^{-\kappa x}$$

for region (II) → $-a < x < a$:

$$V(x) = -V_0$$

Time independent Schrodinger eqn →

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + \frac{2m(E+V_0)}{\hbar^2}\psi = 0$$

$E + V_0 \to +ve$

$\therefore$ Say $l^2 = \frac{2m(E+V_0)}{\hbar^2} > 0$

$\therefore \frac{d^2\psi}{dx^2} + l^2\psi = 0$ → 2nd order ODE with const coefficient.

~~At~~ Ansatz: $\psi \sim e^{rx}$

Aux: $r^2 = -l^2 \to r = \pm il$

General Solution:

$$\psi_{II} = B_1 e^{ilx} + B_2 e^{-ilx}$$

⇒ We have 6 unknown constants – $A_1, A_2, B_1, B_2, C_1, C_2$

(*) In QM: we require the wave-function to be square integrable. i.e. $\int \psi^*\psi\, dx < \infty$

$$\Rightarrow \int_{-\infty}^{-a} \psi_I^*\psi_I\, dx + \int_{-a}^{a} \psi_{II}^*\psi_{II}\, dx + \int_{-a}^{\infty} \psi_{III}^*\psi_{III}\, dx < \infty$$

Given $\psi^*\psi > 0$ for each, ⇒ Each term is individually finite.

(III): $\int_a^\infty \psi_{III}^*\psi_{III}\, dx = \cancel{\int_a^\infty [c_1^* e^{kx} + c_2^* e^{-kx}]^2 dx}$

$$\cancel{= \int_a^a [c_1^2 e^{2kx} + c_2 e^{-2kx} + 2c_1c_2]\, dx}$$

$$= \int_a^\infty [c_1^* e^{kx} + c_2^* e^{-kx}][c_1 e^{kx} + c_2 e^{-kx}]\, dx$$

$$= |C_2|^2 \frac{e^{-2\mathcal{K}a}}{2\mathcal{K}} + \left[\frac{|C_1|^2 e^{2\mathcal{K}x}}{2\mathcal{K}}\right]_0^\infty \longrightarrow \text{Must be zero}$$

$$+ (C_1 C_2^* + C_2 C_1^*)x \Big|_0^\infty$$

We choose $C_1 = 0 \Rightarrow$ Physically allowed solution,

$$\psi_{III} = C_2 e^{-\mathcal{K}x}, \quad \psi_I = A_1 e^{\mathcal{K}x}$$

(*) $\boxed{A5/Q1}$: Show that in the region (I), the square integrability of a wave function implies

$$\psi_I = A_1 e^{\mathcal{K}x}$$

(*) Continuity of $\psi(x)$: (Must match at (I)-(II)-(III) boundaries)

(i) $\underline{x = -a}$:

$$\lim_{h\to 0}\left[\psi_I(-a-h) = \psi_{II}(-a+h)\right]$$

$$\Rightarrow A_1 e^{-\mathcal{K}a} = B_1 e^{-iba} + B_2 e^{ila} \quad -(I)$$

(ii) $\underline{x = a}$:

$$\lim_{h\to 0} \psi_{II}(a-h) = \lim_{h\to 0} \psi_{III}(a+h)$$

$$\Rightarrow B_1 e^{+iLa} + B_2 e^{-iLa} = C_2 e^{-\mathcal{K}a} \quad -(II)$$

(*) Continuity of $\psi'(x)$:

(i) $\underline{x = -a}$:

$$-A\mathcal{K}e^{-\mathcal{K}a} = -iLB_1 e^{-iLa} - iLB_2 e^{iLa}$$

$$\Rightarrow A\mathcal{K}e^{-\mathcal{K}a} = iL\left[B_1 e^{+iLa} \mp B_2 e^{-iLa}\right] \quad -(III)$$

Similarly for

$x = a$:

$$iL\left(B_1 e^{ila} - B_2 e^{-ila}\right) = -\mathcal{K}\, C_2 e^{-\mathcal{K}a} \quad \text{— (IV)}$$

(I)/(II) $\Rightarrow$

$$\frac{A_1}{C_2} = \frac{B_1 e^{-ila} + B_2 e^{ila}}{B_1 e^{ila} + B_2 e^{-ila}} \quad \text{— (V)}$$

(III)/(IV) $\Rightarrow$

$$\frac{A_1}{C_2} = -\frac{B_1 e^{-ila} - B_2 e^{ila}}{B_1 e^{ila} - B_2 e^{-ila}} \quad \text{(VI)}$$

Equating (V) and (VI),

$$\left(B_1 e^{-ila} + B_2 e^{ila}\right)\left(B_1 e^{ila} - B_2 e^{-ila}\right) = -\left(B_1 e^{-ila} - B_2 e^{ila}\right)\left(B_1 e^{ila} + B_2 e^{-ila}\right)$$

$$\Rightarrow B_1^2 = B_2^2$$

$$\Rightarrow \boxed{B_1 = \pm B_2}$$

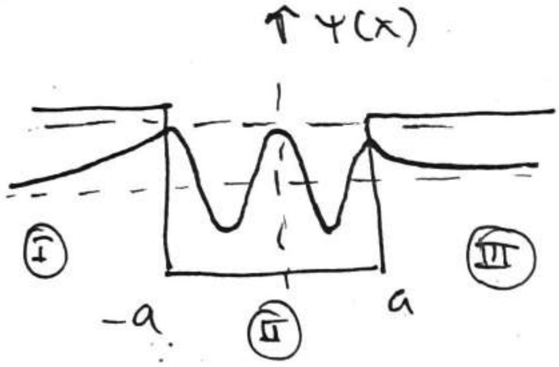
Case $B_1 = B_2$:

$$\psi(x) = \begin{cases} A_1 e^{\mathcal{K}x} \\ 2B_1 \cos(Lx) \\ C_2 e^{-\mathcal{K}x} \end{cases}$$

Now, $\boxed{A_1 = C_2}$ from (V) or (VI),

$$\psi(x) = \begin{cases} A_1 e^{\mathcal{K}x} \\ 2B_1 \cos(Lx) \\ A_1 e^{-\mathcal{K}x} \end{cases}$$

Plotting,



① for $B_1 = B_2$, $\Rightarrow \psi(-x) = \psi(x) \rightarrow$ even function

② For $E < 0$, regions Ⓘ and Ⓘ are classically inacessible.

In QM, both ~~ψ_I and~~ $\psi_I^* \psi_I > 0$ and $\psi^* \psi > 0$

$\Rightarrow$ Non-zero probability of finding the particle.

31st January 2024

⊛ Energy eigenvalues —

We know,

(1) $A_1 e^{-\kappa a} = B_1 \left(e^{ila} + e^{-ila}\right) = 2B_1 \cos(la)$

(3) $\kappa A_1 e^{-\kappa a} = ilB_1 \left(e^{-ila} - e^{ila}\right) = 2lB_1 \sin(la)$

Taking their ratio,

$$\kappa = l \tan(la)$$

We know, $\kappa^2 = -\frac{2mE}{\hbar^2}$, $l^2 = \frac{2m(E+V_0)}{\hbar^2}$

$$\Rightarrow -\frac{2mE}{\hbar^2} = \frac{2m(E+V_0)}{\hbar^2} \tan^2\left(\frac{\sqrt{2ma^2(E+V_0)}}{\hbar}\right)$$

$$\Rightarrow E = -(E+V_0) \tan^2\left(\frac{\sqrt{2ma^2(E+V_0)}}{\hbar}\right)$$

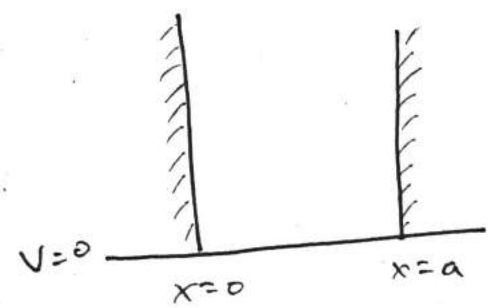
$E = f(E)$ type equation

→ It is a transcendental equation for energy E. It can be solved numerically using a computer.

⊛ Limit of finite sq well to finite sq well →

Infinite sq well —

(A)

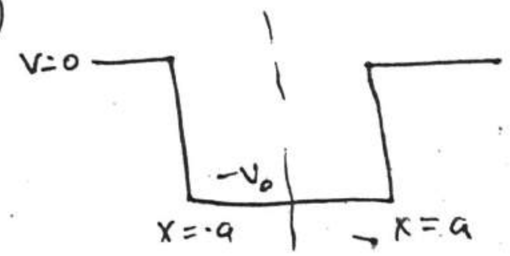


$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

$n = 1, 2, 3,$

(*) Finite sq well —

(B)



(*) How do we go from configeration (B) to (A)

(i) Width: $a \to \frac{a}{2}$

(ii) Shift the origin of Energy: $(E+V_0) \to E$

(iii) Limit: $V_0 \to \infty$

$$E = -(E+V_0)\tan^2\left(\frac{\sqrt{2ma^2(E+V_0)}}{\hbar}\right)$$

(i) $a \to \frac{a}{2}$: $-V_0 + (V_0 + E) =$

$$-(E+V_0)\tan^2\left(\frac{\sqrt{ma^2(E+V_0)/2}}{\hbar}\right)$$

(ii) $(E+V_0) \to E$

$$\frac{V_0}{E} - 1 = \tan^2\left(\frac{\sqrt{ma^2E/2}}{\hbar}\right)$$

(iii) $V_0 \to \infty \Rightarrow$

$$\tan\theta \to \infty$$

$$\Rightarrow \theta = \frac{n\pi}{2}, \quad n = 1, 3, 5, \ldots$$

$$\therefore \frac{ma^2E}{2\hbar^2} = \frac{n^2\pi^2}{4} \Rightarrow E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

$n = 1, 3, 5,$

The other half of the eigenvalues are in the case for $B_1 = -B_2$ (assymetrical)

⊛ Case $B_1 = -B_2$:

wave function, $\psi(x) = \begin{cases} A_1 e^{\kappa x} \\ 2i B_1 \sin(lx) \\ -A_1 e^{-\kappa x} \end{cases}$

$$\psi(-x) = -\psi(x)$$

⊛ $\boxed{A5/Q2}$: Repeat the steps for $B_1 = -B_2$ (as $B_1 = B_2$) and show that the odd wave functions in the infinite square well limit lead to the energy eigenvalue

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}, \quad n = 2, 4, 6, \dots$$

⊛ Class Test – 1 :

Feb 9, 2024 (Friday) at 2 P.M.

$$E = -(E + V_0) \tan^2\left(\frac{\sqrt{2ma^2(E+V_0)}}{\hbar}\right)$$

Case : Deep well (V_0 is large)

$$E_n \simeq -V_0 + \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2}$$

Δ Bound states : An quantum states with negative energy eigenvalue (i.e, $E_n < 0$)
(Assuming energy is zero at infinity)

for deep well : there are finite number of ~~bou~~ bound states.

Case : Shallow well (V_0 is small)

$V_0 \to 0$ so $(E + V_0) \to 0$ as $E < 0$

~~V_0~~ ∴ E must be b/w V_0 and 0

(*) NOT a limit, it is just small

$\theta \to$ small, $\tan\theta \simeq \theta$

$$\therefore\ E = -\frac{2ma^2}{\hbar^2}(E+V_0)^2$$

$$\Rightarrow E^2 + \left(2V_0 + \frac{\hbar^2}{2ma^2}\right)E + V_0^2 = 0$$

Using quadratic formula,

$$E = -\left(V_0 + \frac{\hbar^2}{4ma^2}\right) \pm \sqrt{\left(V_0 + \frac{\hbar^2}{2ma^2}\right)^2 - V_0^2}$$

By construction,

$E + V_0 > 0$, only the +ve root survives.

$$E = -V_0 + \frac{\hbar^2}{4ma^2}\left[\sqrt{1 + \frac{8V_0ma^2}{\hbar^2}} - 1\right]$$

2nd Feb 2024

$$\sqrt{1 + \frac{8V_0ma^2}{\hbar^2}} = 1 + \frac{4V_0ma^2}{\hbar^2} - \frac{1}{8}\left(\frac{8V_0ma^2}{\hbar^2}\right)^2$$

So,

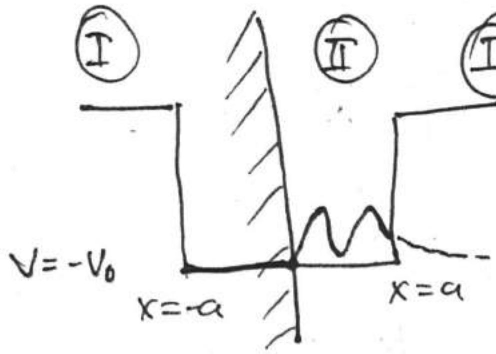
$$E = -V_0 + \frac{\hbar^2}{4ma^2}\left[\sqrt{1 + \frac{8V_0ma^2}{\hbar^2}} - 1\right]$$

$$= -\frac{\hbar^2}{4ma^2}\cdot\frac{1}{8}\left(\frac{8V_0ma^2}{\hbar^2}\right) < 0$$

$\Rightarrow$ It is a bound state.

$\rightarrow$ There is atleast one bound state even for a shallow well.

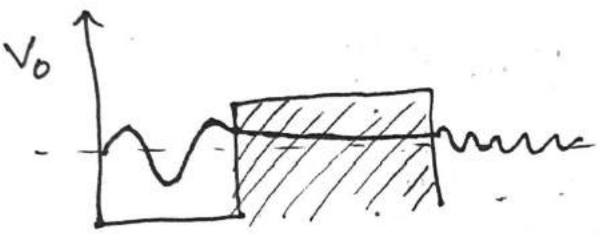
(*) Suppose that the potential well has an infinite wall at $x = 0$ on one side.



→ Solutions are the same as earlier, except with ~~...~~ the new boundary condition

$\psi(x=0) = 0$

→ picks up only the odd functions



• Something might "leak" out of a potential well.

(*) We have seen that trying to measure position causes error in momentum measurement, and vice-versa.

Let us denote :

$\hat{x} \rightarrow$ position operator

$\hat{p} \rightarrow$ momentum operator

$\psi(x) \rightarrow$ an arbitrary wavefunction.

$$\boxed{\hat{p}\,\psi(x) = \frac{\hbar}{i}\frac{d\psi(x)}{dx}}$$

$$\boxed{\hat{x}\,\psi(x) = x\,\psi(x)}$$

Now let us compute commutator,

$$\hat{x}\hat{p}\psi(x) - \hat{p}\hat{x}\psi(x) \qquad \propto \hbar \text{ (we guess)}$$

<u>LHS</u> $\rightarrow \quad \hat{x}(\hat{p}\psi(x)) - \hat{p}.(\hat{x}\psi(x))$

$$= \hat{x}\left(\frac{\hbar}{i}\frac{d\psi}{dx}\right) - \hat{p}(x\psi(x))$$

$$= \frac{\hbar}{i} x \frac{d\psi}{dx} - \frac{\hbar}{i}\frac{d}{dx}(x\psi(x))$$

$$= i\hbar\,\psi(x)$$

Now,

$$(\hat{x}\hat{p} - \hat{p}\hat{x})\psi = i\hbar\psi$$

↳ True $\forall\, \psi$

$$\Rightarrow \boxed{\hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar}$$

(*) Let us define the commutator bracket between two operators, say $\hat{A}$ and $\hat{B}$ as,

$$\boxed{[\hat{A}, \hat{B}] \equiv \hat{A}.\hat{B} - \hat{B}\hat{A}}$$

(*) <u>Canonical commutation relation (CCR)</u> $\rightarrow$

$$\boxed{[\hat{x}, \hat{p}] = i\hbar} \rightarrow$$ <u>First axiom of Quantum Mechanics</u>

Ex: Show that in position representation (x-representation) such that x operator acting on ψ, i.e.,

$$\boxed{\hat{x}\psi = x\psi(x)} \quad \text{(Def of } x \text{ representation)}$$

The general form of the momentum operator is

$$\boxed{\hat{p} = \frac{\hbar}{i}\frac{d}{dx} + f(x)}$$

where f is an arbitrary function.

Proof: Consider,

$$LHS = [\hat{x}, \hat{p}]\psi = \hat{x}\hat{p}\,\psi(x) - \hat{p}\hat{x}\,\psi(x)$$

$$= \hat{x}\left(\frac{\hbar}{i}\frac{d\psi(x)}{dx} + f(x)\psi(x)\right) - \hat{p}\left(x\psi(x)\right)$$

Some algebra $\rightarrow$ $= i\hbar\psi = RHS$

$$\Rightarrow [\hat{x}, \hat{p}] = i\hbar$$

$\longrightarrow$ $\hat{p} = \frac{\hbar}{i}\frac{d}{dx} + f(x)$ is a valid representation that satisfies the CCR.

⊛ $\boxed{\text{A6/Q1}}$ Show that in momentum representation i.e., $\boxed{\hat{p}\psi(p) = p\psi(p)}$, the position operator $\hat{x}$ can be expressed as

$$\boxed{\hat{x}\psi(p) = -\frac{\hbar}{i}\frac{d}{dp}\psi(p) + g(p)\psi(p)}$$

⊛ Simple Harmonic Oscillator (SHO) $\rightarrow$

Newton's eqn $\quad m\ddot{x} = -Kx = -\frac{\partial}{\partial x}$

$$V = \frac{1}{2}Kx.$$

5th Feb 2024

Recall: Simple Harmonic Oscillator. (SHO)

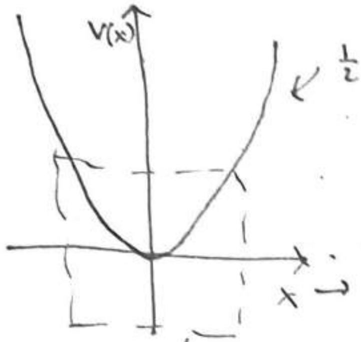
Newton's Law:

$$m\ddot{x} = -\frac{\partial V}{\partial x} \quad , \quad V = \frac{1}{2}Kx^2$$

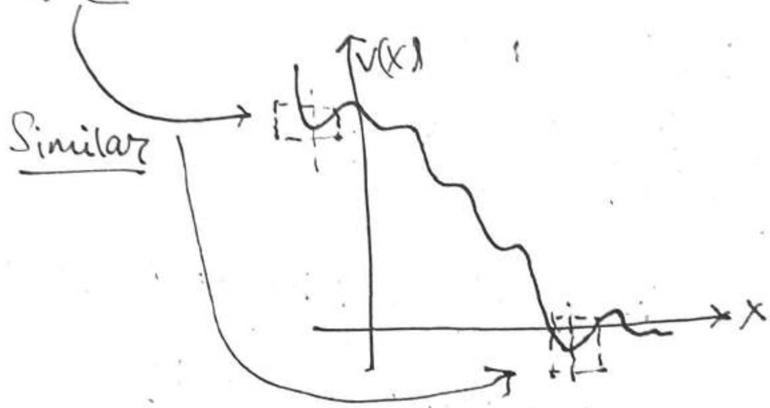
Energy or Hamiltonian of a SHO:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 \quad , \quad \frac{K}{m} = \omega^2$$

Why is SHO problem important physics?



All potential problems where the potential has a finite minima can be approximated as a SHO near its minima.



$$V(X) = V(X_0) + (X-X_0)V'(X_0) + \frac{1}{2!}(X-X_0)^2 V''(X_0) + \cdots$$

(Taylor exp near minima)

$\rightarrow$ At $x = x_0$ (minima) $\Rightarrow V'(x_0) = 0$

$\rightarrow$ $\bar{V}(X) = V(X) - V(X_0)$ define

$$= \frac{1}{2}K(X-X_0)^2$$

Define, $\bar{x} = x - x_0$

$$\Rightarrow \bar{V}(\bar{x}) = \frac{1}{2}K\bar{x}^2 \quad , \quad K = V''(x_0)$$

Quantum SHO problem →

* Time independent Schroedinger equation →

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

But we will not be solving the diff eqn in this method.

* He we shall solve the eigenvalue problem using operator approach by using the CCR directly.

$$[\hat{x}, \hat{p}] = i\hbar$$

Classically,

$$H = \frac{1}{2}m\omega^2\left(x^2 + \frac{p^2}{m^2\omega^2}\right)$$

↳ Remember to always pull out coefficient of x^2

$$\Rightarrow H = \frac{1}{2}m\omega^2\left(x + \frac{ip}{m\omega}\right)\left(x - \frac{ip}{m\omega}\right)$$

$$\Rightarrow H = \frac{1}{2\hbar}m\omega\underbrace{\left(x + \frac{ip}{m\omega}\right)\left(x - \frac{ip}{m\omega}\right)}_{\text{Dimensionless}}\hbar\omega$$

↳ Dim of Energy

Dim of energy

Let us define two operators (dimensionless) —

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right)$$

$$\hat{a}^{+} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right)$$

$\hat{a}^{+}$ is the conjugate of $\hat{a}$.

(*) Let's compute the commutator —

$$[\hat{a}, \hat{a}^{\dagger}] = \left[\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right), \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right)\right]$$

Ex1: Show that $[c_1\hat{A}, c_2\hat{B}] = c_1c_2[\hat{A}, \hat{B}]$

where c_1 and c_2 are complex numbers (Commuting number — 'c' number)

LHS: $[c_1\hat{A}, c_2\hat{B}] = (c_1\hat{A})(c_2\hat{B}) - (c_2\hat{B})(c_1\hat{A})$

$= c_1c_2\hat{A}\hat{B} - c_1c_2\hat{B}\hat{A}$

$= c_1c_2 (\hat{A}\hat{B} - \hat{B}\hat{C})$

$= c_1c_2[\hat{A}, \hat{B}] = \text{RHS}$

Ex2: Show that $[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$

LHS: $[\hat{A}, \hat{B} + \hat{C}] = \hat{A}(\hat{B} + \hat{C}) - (\hat{B} + \hat{C})\hat{A}$

$= \hat{A}\hat{B} + \hat{A}\hat{C} - \hat{B}\hat{A} - \hat{C}\hat{A}$

$= (\hat{A}\hat{B} - \hat{B}\hat{A}) + (\hat{A}\hat{C} - \hat{C}\hat{A})$

$= [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}] = \text{RHS}.$

Using these,

$$[\hat{a}, \hat{a}^{\dagger}] = \left(\frac{m\omega}{2\hbar}\right)\left[\hat{x} + \frac{i\hat{p}}{m\omega}, \hat{x} - \frac{i\hat{p}}{m\omega}\right]$$

$$= \left(\frac{m\omega}{2\hbar}\right)\left([\hat{x}, \hat{x}] + \frac{i}{m\omega}[\hat{p}, \hat{x}] - \frac{i}{m\omega}[\hat{x}, \hat{p}] - \left(\frac{i}{m\omega}\right)^2[\hat{p}, \hat{p}]\right)$$

$= \cancel{\left(\frac{m\omega}{2\hbar}\right)}$

Ex3: Show that $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$

LHS: $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = -(\hat{B}\hat{A} - \hat{A}\hat{B})$

$= -[\hat{B}, \hat{A}]$ = RHS.

Lemma: $[\hat{A}, \hat{A}] = -[\hat{A}, \hat{A}] = 0$

$$[\hat{a}, \hat{a}^{+}] = \left(\frac{m\omega}{2\hbar}\right)\left[-\frac{2i}{m\omega}[\hat{x}, \hat{p}]\right]$$

$$= -\frac{i}{\hbar}[\hat{x}, \hat{p}]$$

$$= -\frac{i}{\hbar}(i\hbar) \quad \text{(using CCR)}$$

$$= 1$$

$$\therefore \boxed{[\hat{a}, \hat{a}] = 1}$$

(*) Consider the product operator $\hat{N} = \hat{a}^{+}\hat{a}$

$$\hat{N} = \hat{a}^{+}\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right)$$

$$= \left(\frac{m\omega}{2\hbar}\right)\left(\hat{x}^2 - \frac{i}{m\omega}\hat{p}\hat{x} + \frac{i}{m\omega}\hat{x}\hat{p} - \left(\frac{i}{m\omega}\right)^2\hat{p}^2\right)$$

$$= \frac{1}{\hbar\omega}\underbrace{\frac{1}{2}m\omega^2\left[\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2}\right)\right.}_{\text{Classical Hamiltonianesque}} + \frac{i}{m\omega}\underbrace{\left.\left(\hat{x}\hat{p} - \hat{p}\hat{x}\right)\right]}_{[\hat{x}, \hat{p}] = i\hbar}$$

$$\hat{N} = \hat{a}^{+}\hat{a} = \frac{1}{\hbar\omega}\hat{H} + \frac{i}{2\hbar}[\hat{x}, \hat{p}]$$

$$\Rightarrow \hat{N} = \hat{a}^{+}\hat{a} = \frac{1}{\hbar\omega}\hat{H} - \frac{1}{2}$$

The Hamiltonian operator $\hat{H} = \left(\hat{N} + \frac{1}{2}\right)\hbar\omega$

$\underline{\text{7th February 2024}}$

Recall : SHO

Define: $$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)$$

$$\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)$$

CCR : $[\hat{x}, \hat{p}] = i\hbar$

$$[\hat{a}, \hat{a}^+] = 1$$

$$\hat{N} \equiv \hat{a}^+\hat{a} = \frac{1}{\hbar\omega}\hat{H} - \frac{1}{2} \Rightarrow \boxed{\hat{H} = \left(\hat{N} + \frac{1}{2}\right)\hbar\omega}$$

What is the physical meaning of $\hat{a}^+$ and $\hat{a}$?

Ex : Show that the ~~pro~~ $[\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$

LHS : $$[\hat{A}\hat{B}, \hat{C}] = (\hat{A}\hat{B})(\hat{C}) - (\hat{C})(\hat{A}\hat{B})$$

$$= \hat{A}\hat{C}\hat{B} - \hat{C}\hat{A}\hat{B} + \hat{A}\hat{B}\hat{C} - \hat{A}\hat{C}\hat{B}$$

$$= (\hat{A}\hat{C} - \hat{C}\hat{A})(\hat{B}) + \hat{A}(\hat{B}\hat{C} - \hat{C}\hat{B})$$

$$= [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$$

$$= RHS.$$

(*) Compute the commutator bracket $[\hat{N}, \hat{a}]$

$$[\hat{N}, \hat{a}] = [\hat{a}^+\hat{a}, \hat{a}]$$

$$= [\hat{a}^+, \hat{a}]\hat{a} + \hat{a}^+[\hat{a}, \hat{a}]$$

$\cancel{= +\hat{a}}$

$$= -[\hat{a}, \hat{a}^+]\hat{a} + 0$$

$$= -1 \cdot \hat{a}$$

$$= -\hat{a}$$

$$\Rightarrow \boxed{[\hat{N}, \hat{a}] = -\hat{a}}$$

(*) Compute,

$$[\hat{N}, \hat{a}^{+}] = [\hat{a}^{+}\hat{a}, \hat{a}^{+}]$$

$$= \hat{a}^{+}[\hat{a}, \hat{a}^{+}] + [\hat{a}^{+}, \hat{a}^{+}]\hat{a}$$

$$= \hat{a}^{+} + 0$$

$$\Rightarrow \boxed{[\hat{N}, \hat{a}^{+}] = \hat{a}^{+}}$$

Let us consider the eigenstates of the operator $\hat{N}$.

$$\boxed{\hat{N}\Psi = n\Psi}$$

(*) We may ask, is the state, say $\phi = \hat{a}\Psi$ an eigenstate of the operator $\hat{N}$

$$\hat{N}\phi = \hat{a}^{+}\hat{a}(\hat{a}\Psi) \Rightarrow \hat{N}\phi = (\hat{N}\hat{a})\cancel{\phi}\Psi$$

$$\Rightarrow \hat{N}\phi = (\hat{N}\hat{a} - \hat{a}\hat{N} + \hat{a}\hat{N})\Psi$$

$$\Rightarrow \hat{N}\phi = ([\hat{N}, \hat{a}] + \hat{a}\hat{N})\Psi$$

$$\Rightarrow \hat{N}\phi = (-\hat{a} + \hat{a}\hat{N})\Psi$$

$$\Rightarrow \hat{N}\phi = -\hat{a}\Psi + \hat{a}(\hat{N}\Psi)$$

$$\Rightarrow \hat{N}\phi = -\phi + n(\hat{a}\phi)$$

$$\Rightarrow \boxed{\hat{N}\phi = (n-1)\phi}$$

(*) Role of $\hat{a}$ is to reduce eigenvalue by 1.

$\Rightarrow$ $\phi = \hat{a}\Psi$ is also an eigenstate of $\hat{N}$ but with eigenvalue reduced exactly by 1.

$\hat{a} \longrightarrow$ Lowering operator or annihilation operator.

⊛ Compute same thing for $\chi = \hat{a}^{+}\psi$

$$\hat{N}\chi = \hat{N}(\hat{a}^{+}\psi) = (\hat{N}\hat{a}^{+})\psi$$
$$= (\hat{N}\hat{a}^{+} - \hat{a}^{+}\hat{N} + \hat{a}^{+}\hat{N})\psi$$
$$= ([\hat{N}, \hat{a}^{+}] + \hat{a}^{+}\hat{N})\psi$$
$$= (\hat{a}^{+} + \hat{a}^{+}\hat{N})\psi$$
$$= \hat{a}\psi + \hat{a}^{+}(\hat{N}\psi)$$
$$= \chi + \hat{a}(n\psi)$$
$$= \chi + n\chi$$
$$= (n+1)\chi$$
$$\Rightarrow \boxed{\hat{N}\chi = (n+1)\chi}$$

→ χ is also an eigenstate but the eigenvalue is raised exactly by 1.

$\hat{a}^{+}$ → Raising operating operator or creation operator.

⊛ What about the states like

$$(\hat{a}\hat{a}\psi) \text{ or } (\hat{a}^{+}\hat{a}^{+}\psi) \ ?$$

$$\hat{N}(\hat{a}\hat{a}\psi) = (n-2)(\hat{a}\hat{a}\psi)$$
$$\hat{N}(\hat{a}^{+}\hat{a}^{+}\psi) = (n+2)(\hat{a}^{+}\hat{a}^{+}\psi)$$

<u>Inconvenient notation</u>

<u>Recall</u>: Inner (Dot) product between two wave-functions $\psi(x)$ and $\phi(x)$:

$$(\phi, \psi) = \langle \phi | \psi \rangle = \int_{L_1}^{L_2} dx\, \phi^*(x) \cdot \psi(x)$$

$$\langle \phi | \cdot | \psi \rangle$$
$$\downarrow \quad \downarrow \quad \downarrow \qquad (???)$$
$$\langle \text{bra} | c | \text{ket} \rangle$$

(Dirac notation)

wave function $\psi \to |\psi\rangle$ is called ket vector

Conjugate (Dual) wave function,

$$\phi^* \longrightarrow \langle \phi |$$

is called a bra vector

Eg: Eigenvalue?

$$\hat{O}\psi = \lambda\psi \Rightarrow \hat{O}|\psi\rangle = \lambda|\psi\rangle$$

Use the eigenvalue to denote the state $|\psi\rangle$

$$\hat{O}|\lambda\rangle = \lambda|\lambda\rangle$$

2 states with λ_1 and λ_2 eigenvalues,

$$\boxed{\begin{aligned} \hat{O}|\lambda_1\rangle &= \lambda_1|\lambda_1\rangle \\ \hat{O}|\lambda_2\rangle &= \lambda_2|\lambda_2\rangle \end{aligned}}$$

$$\hat{N}\psi = n\psi \Rightarrow \hat{N}|n\rangle = n|n\rangle$$

$$\therefore \hat{N}|n-1\rangle = (n-1)|n-1\rangle$$

21st Feb 2024

Dirac notation →

Dot or inner product between two wave functions ψ and ϕ :

$$(\phi, \psi) \equiv \langle \phi , \psi \rangle = \int^{L_2} \psi^* \psi \, dx$$

$\langle \phi | \cdot | \psi \rangle$

$\langle$ bra | (c) | ket $\rangle$

$\psi \to |\psi\rangle$ is called a ket state

Dual (conjugate) wave function

$\psi^* \to \langle \psi | \to$ bra state.

Eigenvalue eqn →

$$\boxed{\hat{O}\psi = \lambda\psi} \quad , \psi \to |\psi\rangle$$

→ In dirac notation

→ $\hat{O}|\psi\rangle = \lambda|\psi\rangle$

It is convenient to use the eigenvalue to denote the state.

$$\hat{O}|\lambda\rangle = \lambda|\lambda\rangle \quad \Big| \; |\psi\rangle \longrightarrow |\lambda\rangle$$

For e.g. : Two different states with different eigenvalues of the operator $\hat{O}$.

$$\hat{O}|\lambda_1\rangle = \lambda_1|\lambda_1\rangle$$

$$\hat{O}|\lambda_2\rangle = \lambda_2|\lambda_2\rangle$$

○ **Normalization** →

$$\text{Squared norm of } \psi = \|\psi\|^2 = (\psi, \psi) = \int_{L_1}^{L_2} \psi^* \psi \, dx$$
$$= \langle \psi | \psi \rangle$$

If ψ is normalized, then,

$$\langle \psi | \psi \rangle = 1 = \|\psi\|^2$$

○ Recasting quantum SHO in Dirac notation →

(*) The action of the operator $\hat{N}$, $\hat{a}$, $\hat{a}^\dagger$

$$\hat{N}\psi = n\psi$$
$$\phi = \hat{a}\psi$$
$$\Rightarrow \hat{N}\phi = (n-1)\psi$$
$$\psi \rightarrow |n\rangle$$
$$\phi \rightarrow |n-1\rangle$$

Complex no.

$$\therefore \boxed{\hat{N}|n\rangle = n|n\rangle}$$

operator   Element of vec space

(*) If $|n\rangle$ is normalized, ~~then,~~ i.e $\langle n|n\rangle = 1$,
then is the ket $|n-1\rangle = \hat{a}|n\rangle$

$\cancel{\langle n-1|an|}, \ \cancel{\langle n-1|n-1\rangle = \langle an|a^\dagger a|n\rangle}$

Sq norm of $|n-1\rangle$ →

$$\langle n-1|n-1\rangle = \langle n-1|(\hat{a}|n\rangle)$$
$$= (\langle n|\hat{a}^\dagger)\cdot(\hat{a}|n\rangle)$$
$$= \langle n|\hat{a}^\dagger\hat{a}|n\rangle$$

$\Rightarrow \langle n-1|n-1\rangle = \langle n|\hat{N}|n\rangle = n\langle n|n\rangle = n$

$\rightarrow |n-1\rangle$ is not normalized.

$|n\rangle, |n-1\rangle$ <u>should</u> be normalized.

In general,

$$\hat{a}|n\rangle = c|n-1\rangle$$

$$\therefore |c|^2 \langle n-1|n-1\rangle = n$$

$$\Rightarrow \boxed{c = \sqrt{n}}$$

$$\therefore \boxed{\hat{a}|n\rangle = \sqrt{n}|n-1\rangle}$$

Now both are normalized.

(*) <u>Raising operator</u> :

$$a^+|n\rangle = c|n+1\rangle$$

Now,

$$|c|^2 \langle n+1|n+1\rangle$$

$$= \langle n|\hat{a}\hat{a}^+|n\rangle$$

$$= \langle n|\{(\hat{a}a^+ - \hat{a}^+\hat{a}) + \hat{a}^+\hat{a}\}|n\rangle$$

$$= \langle n|\{[\hat{a}, \hat{a}^+] + \hat{N}\}|n\rangle$$

$$= \langle n|(1+n)|n\rangle$$

$$= (n+1)$$

$$\therefore \boxed{c = \sqrt{n+1}}$$

$$\Rightarrow \boxed{\hat{a}^+ |n\rangle = \sqrt{n+1}\, |n+1\rangle}$$

So now, $\langle n+1 | n+1 \rangle = 1$

(*) Hamiltonian of $\hat{H}$ →

$$\hat{H} = (\hat{N} + \tfrac{1}{2})\hbar\omega$$

$$\Rightarrow \hat{H}|n\rangle = (\hat{N} + \tfrac{1}{2}\mathbb{I})\hbar\omega |n\rangle$$

$$\Rightarrow \hat{H}|n\rangle = (n + \tfrac{1}{2})\hbar\omega\, |n\rangle$$

if $\hat{H}|n\rangle = E_n |n\rangle$

$$\Rightarrow E_n = (n + \tfrac{1}{2})\hbar\omega$$

$|n\rangle$ kets are also eigenstates of the Hamiltonian operator with eigenvalues,

$$\boxed{E_n = (n + \tfrac{1}{2})\hbar\omega}$$

(*) What is the domain of n?

Inner product : $(\psi, \psi) \geq 0$

$$\langle \psi | \psi \rangle \geq 0 \quad \forall\, |\psi\rangle$$

$$\therefore |\psi\rangle = \hat{a}\,|n\rangle \Rightarrow \langle \psi | \psi \rangle = \langle n | \hat{a}^\dagger \hat{a} | n \rangle$$

$$= n$$

Atleast $n \geq 0$ → a +ve real number.

1st Class → (Copied from Adrika)

23rd Feb 2024

$\hat{a}^{+}$ is a dual operator corresponding to $\hat{a}$.

n is such that $n \geq 0$, $n \in \mathbb{R}$

$\Rightarrow$ $n \to n \in \mathbb{Z}$, $n \to n \notin \mathbb{Z}$

Let us assume that n is not an integer.

Let there be a state $|\alpha\rangle$ where $0 < \alpha < 1$

⊛ Action of lowering operator on α →

$\hat{a}\,|\alpha\rangle \longrightarrow |x\rangle$ → should be a vector with norm-squared positive.

By construction →

$$|x\rangle = \sqrt{\alpha}\,|\alpha - 1\rangle$$

$$\hat{N}\,|\alpha-1\rangle = (\alpha-1)\,|\alpha-1\rangle$$

$$\hat{N}\,|x\rangle = \alpha\,\hat{N}\,|\alpha-1\rangle = (\alpha-1)\left(\sqrt{\alpha}\,|\alpha-1\rangle\right)$$

$$= (\alpha-1)\,|x\rangle$$

Say, we have $|m\rangle$

$$\hat{N}\,|m\rangle = m\,|m\rangle$$

Here, $m = (\alpha - 1)$, which is less than 0.

But we have established $m \geq 0$

Hence our assumption must be wrong.

$\therefore$ n must be ~~an~~ an integer (By contradiction)

(*) In summary, we have established

$$\boxed{\hat{H}|n\rangle = E_n|n\rangle}$$

where $\boxed{E_n = (n+\frac{1}{2})\hbar\omega}$

$n = 0, 1, 2, \ldots$

We have thus solved the SHO solutions without solving Schroedinger's equation..

We are also going to do this using SE, by using Hermite polynomials.

What happens if we chose 2?

$$\hat{a}|2\rangle = \sqrt{2}|1\rangle$$

$$\hat{a}|1\rangle = \sqrt{1}|0\rangle$$

What is $|0\rangle$? It is $|n=0\rangle$

$\Rightarrow$ It is not a null state.

$$\hat{H}|0\rangle = \frac{1}{2}\hbar\omega|0\rangle$$

$$E_0 = \frac{1}{2}\hbar\omega$$

$\Rightarrow$ Energy of QHO must be be $\geq \frac{1}{2}\hbar\omega$

Classically,

- Hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$

Minimum energy $= 0$

But, $\hat{x}, \hat{p} \rightarrow$ cannot both be zero, otherwise we would have violated the uncertainty principle.

Zero-point energy $= \frac{1}{2}\hbar\omega$

Qualitatively, you cannot ever bring something to complete rest.

What happen to the state $|0\rangle$ if we act on it by $\hat{a}$?

$\hat{a}|n\rangle = \sqrt{n}\ |n-1\rangle$

for $n=0$

$\hat{a}|0\rangle = \sqrt{0}\ |0-1\rangle = \phi \rightarrow$ null state.

Since $\sqrt{0}$ is 0.

Thus, we hit null state, we cannot go further down.

Lowering operator $\hat{a}$ annihilated the ground state

$\Rightarrow$ annihilation operator.

Raising operator $\rightarrow$

$$\hat{a}^{+}\ |n\rangle = \sqrt{n+1}\ |n+1\rangle$$

$n=0$

$\hat{a}^{+}\ |0\rangle = \sqrt{0+1}\ |0+1\rangle = |1\rangle$

Thus, we create a higher energy eigenstate starting from the null state (ground state, really).

2nd Class →

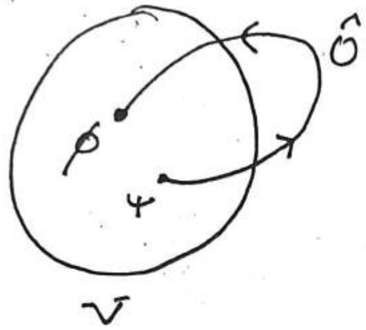
Recall: $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)$

$$\hat{a}^{+} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)$$

$\lambda \xrightarrow{\text{Conjugate}} \lambda^{*}$ (for c-number)

$(x+iy) \xrightarrow{\text{Conjugate}} (x-iy)$

(*) Operator $\hat{O}$ is a map from a vector space V to itself.,
i.e. $\forall$ ~~$\forall$~~ $\psi \in V$, $\psi \xrightarrow{\hat{O}} \phi = \hat{O}\psi$
and $\phi \in V$



$\{\psi\} \rightarrow$ domain of the operator.

(*) ~~Ag~~ Adjoint of an operator →
If given two operators say $\hat{A}$ and $\hat{B}$ satisfy

$$(\phi, \hat{A}\psi) = (\hat{B}\phi, \psi) \quad \forall\ \phi, \psi \in V,$$

then the operator $\hat{B}$ is called the Hermitian ~~co~~ conjugate or the adjoint of the operator $\hat{A}$.
$\hat{B}$ is often denoted as $\hat{A}^{+}$

Ex 1: By using the definition, find the ~~adjoint operator~~ action of the adjoint operator $\hat{O}$ on ψ if $\hat{O}\psi = \lambda\psi$, i.e., $\hat{O}^{+}\psi = ?$

Defn: $(\hat{O}^{+}\phi, \psi) = (\phi, \hat{O}\psi)$

Say, $\phi = \psi$ (arbitrary ϕ and ψ)

$\therefore$ ~~$(\hat{O}^{+}$~~

$\therefore (\hat{O}^{+}\psi = \psi) = (\psi, \hat{O}\psi)$

$$\Rightarrow \int_{-\infty}^{\infty} (\hat{O}^{+}\psi)^{*}\psi\, dx = \int_{-\infty}^{\infty} \psi^{*}(\hat{O}\psi)\, dx$$

$$\Rightarrow \int_{-\infty}^{\infty} (\hat{O}^{+}\psi)^{*}\psi\, dx = \int_{-\infty}^{\infty} \psi^{*}(\lambda^{*})^{*}\psi\, dx$$

$$= \int_{-\infty}^{\infty} (\hat{O}^{+}\psi)^{*}\psi\, dx = \int_{-\infty}^{\infty} (\lambda\psi)^{*}\psi\, dx$$

$$= (\lambda^{*}\psi, \psi)$$

$$\Rightarrow \boxed{\hat{O}^{+}\psi = \lambda^{*}\psi}$$

$$\hat{p} = \frac{\hbar}{i}\frac{d}{dx} \longrightarrow \hat{p}^{+} = -\frac{\hbar}{i}\frac{d}{dx} \text{ ? } \underline{\text{No}}$$

Ex 2. Find the adjoint operator $\hat{O}^{+}$ for the operator $\hat{O} = \frac{d}{dx}$

Defn: $(\hat{O}^{+}\phi, \psi) = (\phi, \hat{O}\psi)$

$$\Rightarrow \int_{-\infty}^{\infty} (\hat{O}^{+} \phi)^{*} \psi dx = \int_{-\infty}^{\infty} \psi^{*} (\hat{O} \psi) dx$$

$$\Rightarrow \int_{-\infty}^{\infty} (\hat{O}^{+} \phi)^{*} \psi dx = \int_{-\infty}^{\infty} \psi^{*} \left(\frac{d}{dx} \psi\right) dx$$

Doing integration by parts on RHS,

$$\int_{-\infty}^{\infty} (\hat{O}^{+} \phi)^{*} \psi dx = \int_{-\infty}^{\infty} dx \left[\frac{d}{dx}(\phi^{*} \psi) - \frac{d\phi^{*}}{dx} \psi\right]$$

$$\Rightarrow \int_{-\infty}^{\infty} dx \, (\hat{O}^{+} \phi)^{*} \psi = \phi^{*} \psi \Big|_{L_1}^{L_2} + \int_{-\infty}^{\infty} dx \left(-\frac{d\phi}{dx}\right)^{*} \psi$$

Term has to go to zero

① Vanishes at boundary

② Periodic boundary condition.

$$\therefore \hat{O}^{+} = -\frac{d}{dx}$$

$\Rightarrow$ momentum is a self-adjoint operator.

(*) A7/Q2 Find the adjoint operator $\hat{p}^{+}$ if

$$\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$$

(*) An operator is called (self-adjoint) or Hermitian

if $\hat{O}^{+} = \hat{O}$

(and domain of $\hat{O}$ = domain of $\hat{O}^{+}$)

(*) In Dirac's bra-ket notation →

$$\hat{O}|\alpha\rangle \quad \| \quad \langle\alpha|\hat{O}^{+}$$

Claim: Eigenvalues of Hermitian operator $\hat{O}$, i.e. $\hat{O}^{+} = \hat{O}$ are real.

Say, $\hat{O}|n\rangle = n|n\rangle$ — (I)

$\langle m|\hat{O}^{+} = \langle m|m^{*}$ — (II)

$\langle m|\cdot$ (I) $\Rightarrow \langle m|\hat{O}|n\rangle = n\langle m|n\rangle$ — (III)

II $\cdot|n\rangle \Rightarrow \langle m|\hat{O}^{+}|n\rangle = m^{*}\langle m|n\rangle$ — (IV)

Subtract (III) from (IV)

$$(m^{*} - n)\langle m|n\rangle = \langle m|\hat{O}^{+}|n\rangle - \langle m|\hat{O}|n\rangle$$
$$= 0$$

$\Rightarrow (n - m^{*})\langle m|n\rangle = 0$

(i) if $m = n$, $\langle n|n\rangle = 1$ (or any other +ve no.)

$\Rightarrow n - n^{*} = 0 \Rightarrow n^{*} = n$

$\Rightarrow$ n must be real.

(ii) If $m \neq n$

$\Rightarrow \boxed{\langle m|n\rangle = 0}$

→ Vectors are orthogonal to each other

⇒ (1) The eigenvalues are real

(2) The eigenstates are orthogonal to each other.

(*) The eigenstates of ~~an~~ a Hermitian operator forms an orthonormal basis set $\{|n\rangle\}$.

$$\hat{N} = \hat{a}^{+}\hat{a} \Rightarrow \hat{N}^{+} = \hat{N}$$

(*) An arbitrary quantum state $|\psi\rangle$ can be expressed as,

$$|\psi\rangle = \sum_n a_n |n\rangle$$

$$\therefore a_n = \langle n|\psi\rangle$$

So,
$$|\psi\rangle = \sum_n a_n |n\rangle$$
$$= \sum_n \langle n|\psi\rangle |n\rangle$$
$$= \sum_n |n\rangle\langle n|\psi\rangle$$

$$\sum_n |n\rangle\langle n| = \mathbb{I}$$

Completeness relation of the basis $\{|n\rangle\}$.

(*) Copied from Subarno's notes. 26th Feb 2024

(*) If $\hat{B} (= \hat{A}^{+}) = \hat{A}$, then it is called a Hermitian operator.

→ Its eigenvalues are real.

→ Eigenvectors form an orthonormal basis.

(*) Expectation value of an operator $\hat{O}$ w.r.t to a state $|\psi\rangle$ is defined as,

$$\langle\psi|\hat{O}|\psi\rangle$$

Ex: Find the expectation value of the Hamiltonian operator $\hat{H}$ w.r.t the state $|n\rangle$

$$\langle n|\hat{H}|n\rangle = \langle n|(\hat{N} + \tfrac{1}{2})\hbar\omega|n\rangle$$

$$= \hbar\omega\langle n|(n+\tfrac{1}{2})|n\rangle$$

$$= (n+\tfrac{1}{2})\hbar\omega$$

$$= E_n$$

(*) In QM, expectation values are physically measurable quantities.

Ex2: Compute the expectation value of the position operator $\hat{x}$ in the eigenstate $|n\rangle$

$$\langle\hat{x}\rangle_{|n\rangle} = \langle n|\hat{x}|n\rangle$$

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)$$

$$\hat{a}^{+} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)$$

$$\Rightarrow \left(\hat{a} + \hat{a}^{\dagger}\right)\sqrt{\frac{\hbar}{2m\omega}} = \hat{x}$$

$$\Rightarrow \langle \hat{x} \rangle_{|n\rangle} = \langle n | \hat{x} | n \rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \langle n | (\hat{a} + \hat{a}^{+}) | n \rangle$$

$$= \left(\sqrt{\frac{\hbar}{2m\omega}}\right)\left(\langle n | \sqrt{n} | n-1 \rangle + \langle n | \sqrt{n+1} | n+1 \rangle\right)$$

$$= 0$$

$$\Rightarrow \langle n | \hat{x} | n \rangle = 0$$

<u>Ex 6</u>: Compute the expectation $\langle n | \hat{x}^2 | n \rangle$

$$\therefore \langle n | \hat{x}^2 | n \rangle = \underbrace{\left(\sqrt{\frac{\hbar}{2m\omega}}\right)^2}_{=m} \langle n | (\hat{a} + \hat{a}^{+})(\hat{a} + \hat{a}^{+}) | n \rangle$$

$$= m \langle n | \hat{a}^2 + \hat{a}^{+}\hat{a} + \hat{a}\hat{a}^{+} + (\hat{a}^{+})^2 | n \rangle$$

$$= m \langle n | \hat{a}^2 + 2\hat{N} - i\hbar + (\hat{a}^{+})^2 | n \rangle$$

$$= m(2n+1) + \langle n | \hat{a}^2 | n \rangle + \langle n | (\hat{a}^{+})^2 | n \rangle$$

$$= m(2n+1) + \langle n | \hat{a} (\sqrt{n} | n-1 \rangle) + \langle n | \hat{a}^{+} (\sqrt{n+1} | n+1 \rangle)$$

Ex: Compute the expectation value of $\hat{p}$ w.r.t $|n\rangle$

$$\langle n|\hat{p}|n\rangle = \left(\sqrt{\frac{\hbar}{2m\omega}}\right)\left(\frac{i}{m\omega}\right) \langle n|(\hat{a}^{+} - \hat{a})|n\rangle = 0$$

Ex: $\langle n|\hat{p}^2|n\rangle$

$$\therefore \langle n|\hat{p}^2|n\rangle = \lambda^2 \langle n|(\hat{a}^{+})^2 - \hat{a}^{+}\hat{a} - \hat{a}\hat{a}^{+} + \hat{a}^2|n\rangle$$

$$= \lambda^2 \langle n|(\hat{a}^{+})^2 - 2\hat{N} - [a,a^{+}] + \hat{a}^2|n\rangle$$

$$= -\lambda^2 (2n+1)$$

$$= -\frac{\hbar}{2m\omega} \cdot \frac{(m\omega)^2}{1} (2n+1)$$

$$= \frac{\hbar m\omega}{2} (2n+1)$$

(*) Variance of the operator:

$$\Delta x^2 = \sigma_x^2 \equiv \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2$$

$$\sigma_p^2 \equiv \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2$$

Product of σ_x^2 and σ_p^2,

$$\sigma_x^2 \sigma_p^2 = \left(\frac{\hbar}{2m\omega}\right)(2n+1)\left(\frac{\hbar m\omega}{2}\right)(2n+1)$$

$$= \frac{\hbar^2}{4}(2n+1)^2$$

$$\Rightarrow \cancel{\sigma_x^2} \quad \boxed{\sigma_x \sigma_p \geq \frac{\hbar}{2}}$$ as min value of $(2n+1)$ is 1

(*) This is the Heisenberg Uncertainty principle.

Copied from Sobarno's notes

1st March 2024

- **Time independent** →

$$\hat{H}\psi_n = E_n \psi_n$$

- **Time-dependent** →

$$i\hbar \frac{dT}{dt} = E_n T(t)$$

$$\Rightarrow \int \frac{dT}{T} = -\frac{iE_n}{\hbar}\int dt$$

$$\Rightarrow T(t) = T(0)\, e^{-i\frac{E_n t}{\hbar}}$$

full solution → (n^{th} eigenvalue)

$$\Psi_n(t;x) = N e^{-\frac{iE_n}{\hbar}t}\,\psi_n(x)$$

N → Normalization const.

$$\Rightarrow |n;t\rangle = e^{-\frac{iE_n t}{\hbar}}|n\rangle$$

General Solution →

$$|\Psi;t\rangle = \sum_{n=0}^{\infty} c_n |n;t\rangle = \sum_{n=0}^{\infty} c_n e^{-\frac{iE_n t}{\hbar}} |n\rangle$$

Norm of $|\Psi, t\rangle$ →

$$\langle \Psi;t|\Psi;t\rangle = \left(\sum_n c_n^* e^{\frac{iE_n t}{\hbar}} \langle m|\right)\left(\sum_m c_m e^{-\frac{iE_m t}{\hbar}} |n\rangle\right)$$

$$= \sum_{m,n} c_n^* c_m e^{i\left(\frac{E_m - E_n}{\hbar}t\right)} \langle m|n\rangle$$

$$\Rightarrow \langle \psi; t | \psi; t \rangle = \sum_{m,n} c_n^* c_m e^{i\left(\frac{E_m - E_n}{\hbar}\right)t} \delta_{mn}$$

$$= \sum_n |c_n|^2 = \langle \psi, 0 | \psi, t=0 \rangle$$

$\therefore$ Time evolution keeps total probability conserved || unitary evolution $\rightarrow$ Inner prod. invariant

$|\psi\rangle \rightarrow A|\psi\rangle$

$|\phi\rangle = A|\phi\rangle$

$$\therefore \langle A\phi | A\psi \rangle = \langle \phi | A^* A | \psi \rangle$$

$$= \langle \phi, \psi \rangle$$

<u>Ex 1</u>: Compute the expectation value

$\langle \psi; t | \hat{x} | \phi; t \rangle$ where

$|\psi; t\rangle = |1; t\rangle$

<u>Proof</u>: $|1; t\rangle = e^{-i\frac{E_n t}{\hbar}}$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^+)$$

$$\therefore \langle 1; t | \hat{x} | 1; t \rangle = \langle 1 | (a + a^+) | 1 \rangle = 0$$

Thus, this $|1, t\rangle$ is a purely quantum mechanical state.

Ex: Compute $\langle \hat{x} \rangle_\psi$ where

$$|\psi;x\rangle = \frac{1}{\sqrt{2}}(|0;t\rangle + |1;t\rangle)$$

Proof: $\langle \psi;x|\hat{x}|\psi;x\rangle$

$$|0;t\rangle = e^{-\frac{iE_0 t}{\hbar}}|0\rangle$$

$$|1;t\rangle = e^{-\frac{iE_1 t}{\hbar}}|1\rangle$$

$$\hat{x}|\psi;x\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(e^{-\frac{iE_0 t}{\hbar}}(a+a^\dagger)|0\rangle + e^{-\frac{iE_1 t}{\hbar}}|1\rangle\right)$$

$$\langle \psi;t|\hat{x}|\psi;x\rangle = \sqrt{\frac{\hbar}{2m\omega}}\frac{1}{\sqrt{2}}$$

$$\left(e^{-\frac{iE_0 t}{\hbar}}(a+a^\dagger)|0\rangle + \langle 0|e^{+i\frac{E_0 t}{\hbar}} + \langle 1|e^{\frac{iE_1 t}{\hbar}}\right)\left((a+a^\dagger)|0\rangle e^{-i\frac{E_0 t}{\hbar}} + (a+a^\dagger)|1\rangle e^{-\frac{iE_1 t}{\hbar}}\right)$$

$$= \overbrace{\langle 0|(a+a^\dagger)|0\rangle}^{=0} + \overbrace{\langle 1|(a+a^\dagger)|1\rangle}^{=0} + e^{\frac{i(E_0-E_1)t}{\hbar}}\langle 0|a+a^\dagger|1\rangle + e^{\frac{i(E_1-E_0)t}{\hbar}}\langle 1|a+a^\dagger|0\rangle$$

$$= \lambda_1(\langle 0|a|1\rangle + \langle 0|a^\dagger|1\rangle) + \lambda_2(\langle 1|a|0\rangle + \langle 1|a^\dagger|0\rangle)$$

$$= \lambda_1(\langle 0|0\rangle + \langle 0|a^\dagger|1\rangle) + \lambda_2(\langle 1|0\rangle + \langle 1|1\rangle)$$

$$= \lambda_1 + \lambda_2$$

$$= \left(\sqrt{\frac{\hbar}{2m\omega}}\right)\left(\frac{1}{2}\right)\left[e^{i\frac{(E_0-E_1)t}{\hbar}} + e^{i\frac{(E_1-E_0)t}{\hbar}}\right.$$

We know, ~~$E_0 - E_1 = \hbar\omega$~~

$$E_1 - E_0 = \hbar\omega$$

$$\therefore \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{1}{2}\right)\left[e^{i\omega t} + e^{-i\omega t}\right]$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{1}{2}\right)\cos(\omega t)$$ ⊛ Clarify these notes

⊛ $\boxed{A8/Q1}$ Show $\langle \psi; t|\hat{p}|\psi; t\rangle$

$$= \sqrt{\frac{m\omega\hbar}{2}}\sin(\omega t)$$

$$p = m\frac{dx}{dt}$$

$$\langle \hat{p}\rangle = -m\frac{d}{dt}\langle \hat{x}\rangle$$

6th March 2024

<u>Recall</u>: for a given $|\psi\rangle = \frac{1}{\sqrt{2}}(|0;t\rangle + |1;t\rangle)$

$$\langle \psi|\hat{x}|\psi\rangle = \langle \hat{x}\rangle_\psi = \sqrt{\frac{\hbar}{2m\omega}}\cos\omega t$$

and $\langle \hat{p}\rangle_\psi = \langle \psi|\hat{p}|\psi\rangle = -\sqrt{\frac{m\omega\hbar}{2}}\sin\omega t.$

We know classically that,

$$\boxed{p = m\frac{dx}{dt}}$$

⊛ We note that,

$$\boxed{m\frac{d}{dt}\langle \hat{x}\rangle_\psi = \langle \hat{p}\rangle_\psi}$$

We also know that,

$$\frac{dp}{dt} = F = -Kx = -m\omega^2 x$$

We can also see that, Similar

$$\frac{d}{dt} \langle \hat{p} \rangle_\psi = -m\omega^2 \langle \hat{x} \rangle$$

There are states in QMech in which expectation values of $\hat{x}$, $\hat{p}$ shows similar properties as classical mechanics.

→ Quantum to classical correspondence

→ Ehrenfest theorem

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|0;t\rangle + |1;t\rangle \right)$$

$$\Rightarrow |\psi\rangle = \frac{1}{\sqrt{2}} \left(e^{-\frac{iE_0 t}{\hbar}} |0\rangle + e^{-\frac{iE_1 t}{\hbar}} |1\rangle \right)$$

→ This is an example of a so-called wave packet. → a linear combination of two or more basis states

You can have a linear combination of as many states as possible as long as

$$\langle \psi | \psi \rangle < \infty$$

$$\Rightarrow \sum_n |c_n|^2 < \infty$$

Schroedinger eqn :

Energy eigenfunc

$$\boxed{\hat{H}\,\Psi_n(x) = E_n\,\Psi_n(x)}$$

How to relate them?

Operator method

$$\boxed{\hat{H}\,|n\rangle = E_n\,|n\rangle}$$

kets

* Relation b/w $|n\rangle$ and $\Psi_n(x)$:

$\hat{A} \rightarrow$ vector.

What is the 'x' component of the vector A?

$$A_x = (\hat{e}_x, \hat{A})$$

We take the dot

$$= \langle \hat{e}_x, \hat{A} \rangle$$

Similarly

$$\boxed{\Psi_n(x) = \langle x | n \rangle}$$

* Action of $\hat{x}$ and $\hat{p}$ on position basis ket $|x\rangle$

So in this basis, by def, ~~sho~~ $\hat{x}$ should act as eigenvalue expression

$$\hat{x}\,|x\rangle = x\,|x\rangle$$

$$\hat{p}\,|x\rangle = \frac{\hbar}{i}\frac{d}{dx}\,|x\rangle$$

We find duals of this,

$$\langle x|\hat{x} = \langle x|\,x$$

$$\langle x|\hat{p} = \langle x|\,\frac{\hbar}{i}\frac{d}{dx} = \frac{\hbar}{i}\frac{d}{dx}\langle x|$$

as $\hat{x}$ and $\hat{p}$ are Hermitian.

Ground State :

$$|0\rangle \rightarrow \psi_0(x) = \langle x|0\rangle$$

We know that, $\hat{a}|0\rangle = 0$ (Null)

$$\Rightarrow \langle x|\hat{a}|0\rangle = 0$$

$$\Rightarrow \langle x|\hat{x} + \frac{i}{m\omega}\hat{p}|0\rangle = 0$$ as they are c-num

$$\Rightarrow x\langle x|0\rangle + \frac{i}{m\omega}\frac{\hbar}{i}\cancel{\langle x}\frac{d}{dx}\langle x|0\rangle = 0$$

$$\Rightarrow x\,\psi_0(x) + \frac{\hbar}{m\omega}\frac{d}{dx}\psi_0(x) = 0$$

$$\Rightarrow \frac{d\psi_0}{\psi_0} = -\frac{m\omega}{\hbar}x\cdot dx$$

$$\Rightarrow \ln\psi_0 = -\frac{m\omega}{\hbar}x^2 + c$$

$$\rightarrow \boxed{\psi_0(x) = N e^{-\frac{m\omega}{2\hbar}x^2}}$$

Gaussian

Does this satisfy Schroedinger eqn?

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_0}{dx^2} + \frac{1}{2}m\omega^2x^2\psi_0 = E\psi_0$$

$$\psi_0' = Ne^{-\frac{m\omega}{2\hbar}x^2}(2x)\left(-\frac{m\omega}{2\hbar}\right)$$

$$\psi_0'' = Ne^{-\frac{m\omega}{2\hbar}x^2}\left(-\frac{m\omega}{2\hbar}\right) + N(2x)\left(-\frac{m\omega}{2\hbar}\right)e^{-\frac{m\omega}{2\hbar}x^2}(2x)\left(-\frac{m\omega}{2\hbar}\right)$$

$\Rightarrow \psi_0'' = \mathcal{N} e^{-\frac{m\omega}{2\hbar}x^2}\left(-\left(\frac{m\omega}{\hbar}\right) + \left(\frac{m\omega}{\hbar}\right)^2 x^2\right)$

$\Rightarrow E = \frac{\hbar\omega}{2} - \frac{1}{2}m\omega^2 x^2 + \frac{1}{2}m\omega^2 x^2 = \frac{1}{2}\hbar\omega$

$\Rightarrow \psi_0(x)$ is a solution of Schroedinger equation with $E = \frac{1}{2}\hbar\omega$

$\psi_0(x) \rightarrow$ is the ground state.

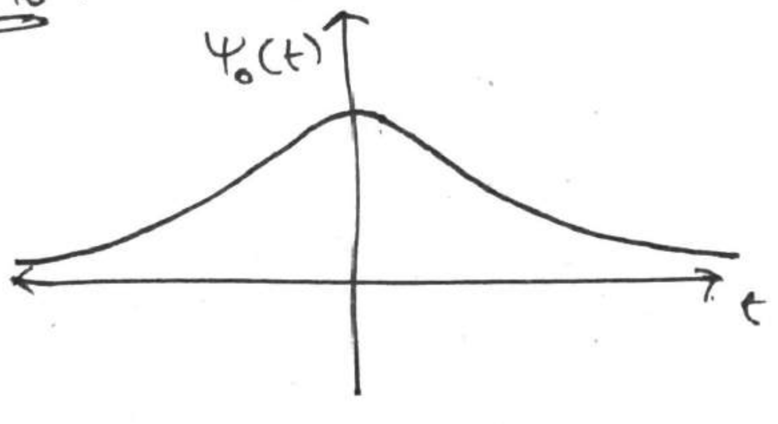
* $\boxed{\text{A8/Q2}}$ Show that the normalization constant $\mathcal{N}$ for the state

$\psi_0(x) = \mathcal{N}$ for the state

$\psi_0(x) = \mathcal{N} e^{-\frac{m\omega}{2\hbar}x^2}$

is $\mathcal{N} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$

<u>Plotting ψ_0:</u>



→ No node

→ 0 at $-\infty$ and $+\infty$

→ Ground state.

⊛ What is the position representation (x-repr) of the ket $|1\rangle$?

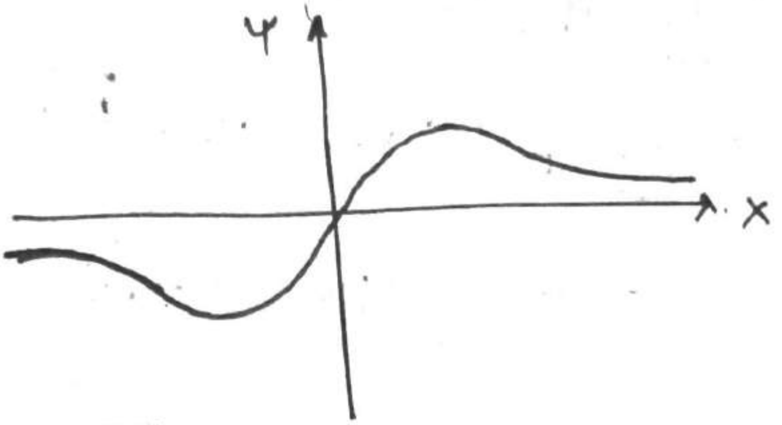
$$|1\rangle = \hat{a}^{+}|0\rangle$$

$$\psi_1(x) = \langle x|1\rangle = \langle x|\hat{a}^{+}|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\langle x|\hat{x} - \frac{i}{m\omega}\hat{p}|0\rangle$$

$$\Rightarrow \psi_1(x) = \sqrt{\frac{m\omega}{2\hbar}}\Big[x\underbrace{\langle x|0\rangle}_{=\psi_0} - \frac{\hbar}{m\omega}\frac{d}{dx}\underbrace{\langle x|0\rangle}_{\psi_0}\Big]$$

$$= \sqrt{\frac{m\omega}{2\hbar}}\left[x\psi_0 - \frac{\hbar}{m\omega}\frac{d\psi_0}{dx}\right]$$

$$\Rightarrow \psi_1(x) = N x e^{-\frac{m\omega}{2\hbar}x^2}$$



⊛ $\boxed{A8/Q3}$ Using Schroedinger equation verify that $\psi_1(x)$ is a solution with energy eigenvalue $E = \frac{3}{2}\hbar\omega$

⊛ 1 classtest before Spring break.

8th March 2024

Recall: $\boxed{\hat{H}|n\rangle = E_n|n\rangle}$

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

$$|n;t\rangle = e^{-i\frac{E_n t}{\hbar}}|n\rangle$$

→ c-number.

$$\hat{H}|n;t\rangle = e^{-i\frac{E_n t}{\hbar}}\hat{H}|n\rangle$$

$$= E_n\left(e^{-iE_n t/\hbar}|n\rangle\right)$$

$$= E_n|n;t\rangle$$

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0;t\rangle + |1;t\rangle\right)$$

$$\hat{H}|\psi\rangle = \frac{1}{\sqrt{2}}\left(\hat{H}|0;t\rangle + \hat{H}|1;t\rangle\right)$$

$$= \frac{1}{\sqrt{2}}\left(E_0|0;t\rangle + E_1|1;t\rangle\right)$$

$$= \frac{1}{\sqrt{2}}\frac{\hbar\omega}{2}\left(|0;t\rangle + 3|1;t\rangle\right) \neq \frac{1}{\sqrt{2}}\frac{\hbar\omega}{2}|\psi\rangle$$

Not an eigenfunction.

(*) Destroys the original state — So how do we find the energy of wavepacket? (Not eigenval anymore)

Ex: Compute the expectation value of the Hamiltonian op $\hat{H}$ in the state $|\psi\rangle$

$$\langle \hat{H} \rangle_\psi = \langle \psi | \hat{H} | \psi \rangle$$

$$= \frac{1}{\sqrt{2}} \left(\langle 0;t| + \langle 1,t| \right) \cdot \frac{1}{\sqrt{2}} \left(E_0 |0,t\rangle + E_1 |1,t\rangle \right)$$

$$= \frac{1}{2}(E_0 + E_1) = \hbar\omega$$

(*) As the eigenstates are normalized and are orthogonal to each other at all times.

Here we end SHO.

$$P \xrightarrow[\text{comp}]{\text{Do not}} \hat{P}$$

$\hat{P}$ $\downarrow |\psi\rangle$ $\rightarrow$ Initial values encoded here.

$P \leftrightarrow$ comparable $\leftrightarrow \langle \hat{P} \rangle_\psi$ expectation w.r.t state

○ <u>Free particles in QM</u> $\rightarrow$ (1+1 dim)

NLM 2: $\boxed{m \frac{d^2x}{dt^2} = F}$

If force is absent, we call it free particle.

i.e, if $F = 0$, then the particle is called a free particle.

$$F = -\frac{\partial V}{\partial x} = 0 \Rightarrow V = V_0$$

$\therefore$ In QM we still have a free parameter of V.

By convention, we choose it to be zero, i.e,

$V_0 = 0$

(*) **Hamiltonian:**

$$\boxed{H = \frac{p^2}{2m}}$$

Solving NLM, we have,

$v = \text{const}.$

$x = v_0 t + x_0$

So what is the probability of finding the particle at some point in space?

It can be anywhere, ~~ax~~ as t varies and x_0 could be anything

This causes a problem (??)

(*) **QM:** Time-independent Schroedinger eqn

$$\hat{H}\psi(x) = E\psi(x)$$

$$\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$$

$$\therefore \; -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \Rightarrow \frac{d^2\psi}{dx^2} + k^2\psi = 0$$

$$\Rightarrow k^2 = \frac{2mE}{\hbar^2}$$

Ansatz: $\psi \sim e^{rx}$

$$\Rightarrow r^2 + k^2 = 0 \Rightarrow \boxed{r = \pm ik}$$

Gen. Solution (time indep):

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad E = \frac{\hbar^2 k^2}{2m}$$

(*) <u>Time - dependent part of Schr. equ:</u>

$$i\hbar \frac{dT}{dt} = ET$$

$\Rightarrow \Psi(x,t) = T(t)\,\psi(x)$ (using this)

$$\therefore T(t) = e^{-\frac{iE}{\hbar}t}\,T(0)$$

Define, $\frac{E}{\hbar} = \omega$

$$\therefore \boxed{T(t) = e^{-i\omega t}\,T(0)}$$

Combining to get full solution,

<u>full solution of SE</u> $\rightarrow$

$$\psi(t,x) = T_0 e^{-i\omega t}\left(Ae^{ikx} + B^{-ikx}\right)$$

$$\Rightarrow \boxed{\psi(t,x) = A_0 e^{-i(\omega t - kx)} + Be^{-i(\omega t + kx)}}$$

$\hookrightarrow$ waves (or particle ?)

$e^{-i(\omega t - kx)} \rightarrow$ A moving wave from left to right as t increases.

$e^{-i(\omega t + kx)} \rightarrow$ A moving wave from right to left as t increases.

(*) How do we determine A and B?

Sq. Norm of $\psi(t,x) \rightarrow$

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

$$\Rightarrow \|\Psi(t,x)\|^2 = \int_{-\infty}^{\infty} (|A|^2 + |B|^2)\,dx + \int_{-\infty}^{\infty} dx\,\left[AB^* e^{2ikx} + A^* B e^{-2ikx}\right]$$

$$\Rightarrow \|\Psi(t,x)\|^2 = (|A|^2+|B|^2)\int_{-\infty}^{\infty} dx + (AB^* + A^*B)\int_{-\infty}^{\infty} dx\, e^{i2kx}$$

Oscillating

Goes to ∞
But cannot be killed
as $A = B = 0$ required

$\hookrightarrow < \infty$

$\Rightarrow$ There is no solution of free particle in SE in Hilbert Space.

$$\Rightarrow \boxed{\|\Psi(t,x)\|^2 \nless \infty}$$

$\hookrightarrow$ wave function Ψ is not normalizable.
i.e. it is not part of Hilbert Space.

(*) Free particle is a pathological ~~inte~~ system for QM.

<u>For SHO, we had,</u>

$$\hat{H}|n\rangle = E_n |n\rangle$$

$$\langle n|m\rangle = \delta_{nm} \quad \text{(Kronecker Delta)}$$

$$\sum_n |n\rangle\langle n| = \mathbb{I} \quad \text{(Completeness relation)}$$

$$\langle x|n\rangle = \Psi_n(x)$$

$\hat{H}\,\psi(x) = E_k \psi(x)$

$$E_k = \frac{\hbar^2 k^2}{2m}$$

These are analogies to SHO.

$\hat{H}\,|k\rangle = E_k\,|k\rangle$

$|k\rangle$ ket in x-repr.

Now, what is the analogy of the ~~completeness~~

$\langle n|m\rangle = \delta_{nm}$?

Note that the continuous ext of the completeness relation (Sturm-Louiville) holds.

$\sum |n\rangle\langle n| = \mathbb{I}$ and $\int_{-\infty}^{\infty} dx\, |x\rangle\langle x| = \mathbb{I}$

$$\therefore \langle k'|k\rangle = \langle k'|\mathbb{I}|k\rangle$$

$$= \int_{-\infty}^{\infty} dx\, \underbrace{\langle k'|x\rangle}_{\psi^*_{k'}} \underbrace{\langle x|k\rangle}_{\psi_k}$$

$$= \int_{-\infty}^{\infty} dx\, \psi^*_{k'}(x)\, \psi_k(x)$$

$$= \int_{-\infty}^{\infty} dx\, e^{-i(k-k')x}$$

$$= \delta(k-k')$$

(*) <u>Dirac delta</u> →
- It is a distribution.
- It is not a function.

△ **Def:** $\int d\mathbf{r}\, f(\mathbf{r})\, \delta(\mathbf{r}-\mathbf{r}') = f(\mathbf{r}')$

$$\delta(\mathbf{r}-\mathbf{r}') = 0 \text{ if } \mathbf{r} \neq \mathbf{r}'$$

Δ **Def:** $\int d\mathcal{R}\, f(\mathcal{R})\, \delta(\mathcal{R}-\mathcal{R}') = f(\mathcal{R}')$

$$\delta(\mathcal{R}-\mathcal{R}') = 0 \text{ if } \mathcal{R} \neq \mathcal{R}'$$

11th March 2024

Free particles in QM $\rightarrow$

Recall: $\hat{H}|k\rangle = E_k|k\rangle$ with $E_k = \dfrac{\hbar^2 k^2}{2m}$

$\hat{H}|n\rangle = E_n|n\rangle$

$\langle m|n\rangle = \delta_{mn}$

$\sum_n |n\rangle\langle n| = \mathbb{I}$

But for free particles,

$\psi^*\psi$ is not normalizable

$$\hat{H} = \frac{\hat{p}^2}{2m}$$

Analogy: $|n\rangle$ is an abstract vector

$\vec{A}$ (random vector)

If we project this in all directions, and then recombine the set of all components (complete set of bases), we should be able to reconstruct $\vec{A}$.

$$\sum |n\rangle\langle n| = \mathbb{I} \Longrightarrow \int dx\, |x\rangle\langle x| = \mathbb{I} \text{ or } 1$$

$$\therefore |\psi\rangle = \mathbb{I}|\psi\rangle$$

$$\Rightarrow \sum_n |n\rangle\langle n|\psi\rangle = \sum_n c_n|n\rangle$$

$\vec{n}$ is the direction of the random vector and the summation of $\sum_n |n\rangle\langle n|$ is over countably infinite elements (infinite dimensions) x-rep of $|K\rangle$

$$\psi_K(x) = \langle x|K\rangle = e^{-iKx}$$

$$\langle k'|k\rangle = \int dx\, e^{-i(k-k')x}$$

$$= \delta(k-k') = \delta(k,k')$$

Dirac Delta.

① $\delta(k-k') = 0$ if $k \neq k'$

② $\int dk\, f(k)\, \delta(k-k') = f(k')\ \forall f(k)$

for $f(k) = 1$

$$\Rightarrow \int_{-\infty}^{\infty} dk\, \delta(k-k') = 1 \Big\}\ \text{also valid over } k+\epsilon \text{ and } k-\epsilon$$

(*) Note: It is a distribution, not a function.

As for the free particle, we do not gain any more information from this notation, taking $(-\infty, \infty)$ as limits.

However, we can solve the free particle by claiming that the universe is not finite:

$\longrightarrow$ Particle in a 'very' large box.

$$\langle k|k'\rangle = \int_{-L}^{L} dx\, e^{-i(k-k')x}$$

$$= -2L\, \delta_{k,k'}$$

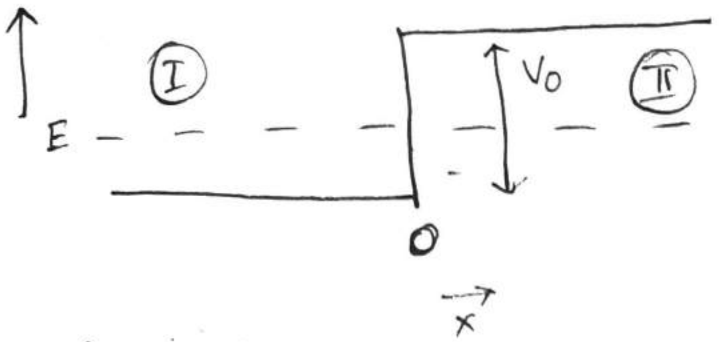
$$\boxed{\psi_k(L) = \psi_k(-L) = 0}$$

$$\therefore \langle x|k\rangle = \frac{1}{\sqrt{2L}} e^{-ikx}$$

CT2: Mar 18, 2024 (Monday)

Coming back to our discussion on Newtonian QM, we now study,

(*) Scattering and Tunnelling phenomena →



$$V = \begin{cases} 0, & x < 0 \\ V_0, & x \geq 0 \end{cases}$$

Region (I): $\dfrac{-\hbar^2}{2m} \dfrac{d^2\psi}{dx^2} = E\psi$, $\boxed{E > 0}$

$\Rightarrow \psi = Ae^{ikx} + Be^{-ikx}$, $k^2 = \dfrac{2mE}{\hbar^2}$

Region (II) →

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V_0\psi = E\psi \quad , E > 0$$

$$\Rightarrow \frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} = (E - V_0)\psi$$

↳ $E < V_0$ Bound state problem.

Case A: $\dfrac{d^2\psi}{dx^2} + \dfrac{2m(E-V_0)}{\hbar^2}\psi = 0$

$$\Rightarrow \boxed{l^2 = \frac{2m(V_0 - E)}{\hbar^2} > 0}$$

$$\psi_{II}(x) = Ce^{lx} + De^{-lx}$$

If we demand normalizability, $C = 0$

$$\psi_{II}(x) = De^{-lx}$$

$|\psi_{II}|^2 > 0 \quad \forall x$

This phenomena of finding the particle even in classically prohibited regions is called tunnelling.

Ex: Spontaneous decay of atomic nucleus (radioactive)

Nucleus

Not explainable using CM,
but explained by tunnelling.
(Spontaneous and random)

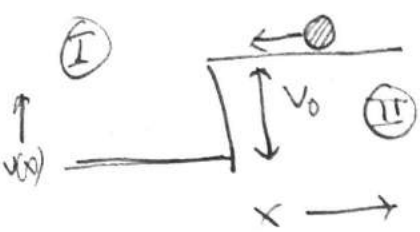
This phenomena of finding the particle even in classically prohibited regions is called ~~tune~~ tunnelling.

Ex: Spontaneous decay of atomic nucleus (radioactive)

Nucleus

Not explainable using CM, but explained by tunnelling. (Spontaneous and random)

13th March 2024



QM predicts that the particle can be scattered backwards too.

Case B: $E > V_0$: $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi$

Say $l^2 = \frac{2m(E-V_0)}{\hbar} > 0$

$\psi_{II} = Ce^{ilx} + De^{-ilx}$

Time dependent →

$$\Psi_I(t,x) = e^{-i\omega t}\left(Ae^{ikx} + Be^{-ikx}\right)$$

$$\Psi_{II}(t,x) = e^{-i\omega t}\left(Ce^{ilx} + De^{-ilx}\right)$$

Is it possible to have only right to left moving waves in both regions ~~I and~~ I and II

↳ Can we set both A and C to zero?

Continuity → $\psi_I(0) = \psi_{II}(0) \Rightarrow \boxed{A+B = C+D}$ — (I)

$\psi_I'(0) = \psi_{II}'(0) \Rightarrow \boxed{k(A-B) = l(C-D)}$ — (II)

$l \times (1) + (2) \Rightarrow C = \frac{A}{2}\left(1+\frac{k}{l}\right) + \frac{B}{2}\left(1-\frac{k}{l}\right)$

$l \times (1) - (2) \Rightarrow D = \frac{A}{2}\left(1-\frac{k}{l}\right) + \frac{B}{2}\left(1+\frac{k}{l}\right)$

If $A = 0 = C$
$\Rightarrow B = 0 = D$
(Trivial)

For non-trivial solution of Ψ,

$R = L \Rightarrow \boxed{V_0 = 0}$

In QM, if there is difference in potential there will be scattering.

O Quantum mechanics in 3D →

3D ⇒ (3 space + 1 time)

In 1D:

Canonical Commutation relation (CCR)

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar$$

$\hat{x} \rightarrow$ position operator

$\hat{p} \rightarrow$ momentum operator.

In 3D:

Not operator

Position vector (Classical) $\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$

Use index notation: $\begin{cases} r_1 = x, \; r_2 = y, \; r_3 = z \\ \hat{e}_1 = \hat{i}, \; \hat{e}_2 = \hat{j}, \; \hat{e}_3 = \hat{k} \end{cases}$

$$\vec{r} = r_1\hat{e}_1 + r_2\hat{e}_2 + r_3\hat{e}_3$$

$$\Rightarrow \boxed{\vec{r} = \sum_{i=1}^{3} r_i \hat{e}_i}$$

Momentum vector:

$$\boxed{\vec{p} = \sum_{i=1}^{3} p_i \hat{e}_i}$$

$p_1 = p_x$

$p_2 = p_y$

$p_3 = p_z$

⊛ CCR in 3D →

$\boxed{[\hat{x}, \hat{p}_x] = i\hbar}$, $\boxed{[\hat{y}, \hat{p}_y] = i\hbar}$

$\boxed{[\hat{z}, \hat{p}_z] = i\hbar}$

Photon argument

Also, independence of directions,

$$[\hat{x}, \hat{P}_y] = 0 = [\hat{x}, \hat{P}_z]$$

and so on.

Same argument.

Also,

$$[\hat{P}_x, \hat{P}_y] = 0 = [\hat{P}_y, \hat{P}_z]$$

and

$$[\hat{x}, \hat{y}] = 0 = [\hat{y}, \hat{z}]$$

(Some thing about Space time stretching, idk)

In index notation,

$$\boxed{[\hat{r}_i, \hat{P}_j] = i\hbar\delta_{ij}} \quad \boxed{[\hat{r}_i, \hat{r}_j] = 0 = [\hat{P}_i, \hat{P}_j]},$$

CCR in 3D

* Angular momentum →

$$\boxed{\vec{L} = \vec{r} \times \vec{p}}$$ Classical

In index notation,

$$\boxed{L_i = \sum_{j,k=1}^{3} \epsilon_{ijk} r_j P_k} \quad \boxed{\begin{array}{l} L_1 = L_x \\ L_2 = L_y \\ L_3 = L_z \end{array}}$$

* ϵ_{ijk} : Levi-Civita symbol:

$$\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = +1$$

$$\epsilon_{321} = \epsilon_{213} = \epsilon_{132} = -1$$

$$\epsilon_{ijk} = 0 \quad \text{if } i = j \text{ or } j = k \text{ or } k = i$$

Cyclically permute to get increasing or decreasing seq.

$$L_x = L_1 = \sum_{j,k=1}^{3} \epsilon_{ijk} r_j P_k = \epsilon_{123} r_2 P_3 + \epsilon_{132} r_3 P_2$$

$$\boxed{L_x = y P_z - z P_x}$$

(*) $\boxed{A9/Q1}$ Using Levi-civita symbol show that $L_y = z p_x - x p_z$ and $L_z = x p_y - y p_x$

Filling in notes. (Piyush's Notes)

Say, we define the form of angular momentum operator as

$$\hat{L}_x = \hat{y}\,\hat{P}_z - \hat{z}\,\hat{P}_y$$

Quantum operator corresponding to the x- component of $\vec{L}$ [classical]

(*) Hermitian Conjugate :

$$\hat{L}_x^{+} = (\hat{y}\,\hat{P}_z)^{+} - (\hat{z}\,\hat{P}_y)^{+}$$

$$= \hat{P}_z^{+}\,\hat{y}^{+} - \hat{P}_y^{+}\,\hat{z}^{+}$$

Since, $\hat{x}$, $\hat{P}_x$ are self adjoint [Hermitian]

$$\Rightarrow \hat{P}_z\,\hat{y} - \hat{P}_y\,\hat{z}$$

~~Since~~ $\cancel{\Rightarrow [\hat{P}_z\,\hat{y} - \hat{P}_y\,\hat{z}]}$

Since $[\hat{P}_z, \hat{y}] = 0 \Rightarrow \hat{P}_z$ and $\hat{y}$ commute.

$$\Rightarrow \hat{y}\,\hat{P}_z - \hat{z}\,\hat{P}_y$$

$$\Rightarrow \boxed{\hat{L}_x^{+} = \hat{L}_x} \longrightarrow \text{Self adjoint [Hermitian]}$$

Eigenvalues of angular momentum operators $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ are reals.

Ex: Compute the commutator bracket

$$[\hat{L}_x, \hat{L}_y] = [\hat{y}\,\hat{P}_z - \hat{z}\,\hat{P}_y, \hat{z}\,\hat{P}_x - \hat{x}\,\hat{P}_z]$$

$$= [\hat{y}\,\hat{P}_z, \hat{z}\,\hat{P}_x] - [\hat{z}\,\hat{P}_y, \hat{z}\,\hat{P}_x] - [\hat{y}\,\hat{P}_z, \hat{x}\,\hat{P}_z] + [\hat{z}\,\hat{P}_y, \hat{x}\,\hat{P}_z]$$

$$= \left[(\hat{y}\hat{p}_z)(\hat{z}\hat{p}_x) - (\hat{z}\hat{p}_x)(\hat{y}\hat{p}_z) \right] - \left[(\hat{z}\hat{p}_y)(\hat{z}\hat{p}_x) - (\hat{z}\hat{p}_x)(\hat{z}\hat{p}_y) \right]$$

$$- \left[(\hat{y}\hat{p}_z)(\hat{x}\hat{p}_z) - (\hat{x}\hat{p}_z)(\hat{y}\hat{p}_z) \right]$$

$$= \left[\hat{y}(\hat{p}_z \hat{z})\hat{p}_x - \hat{y}(\hat{z}\hat{p}_z)\hat{p}_x \right] - \hat{z}\left[\hat{p}_y \hat{p}_x - \hat{p}_x \hat{p}_y \right]\hat{z}$$

$$- \hat{p}_z \left[\hat{y}\hat{x} - \hat{x}\hat{y} \right]\hat{p}_z + \left[\hat{x}(\hat{z}\hat{p}_z)\hat{p}_y - \hat{x}(\hat{p}_z\hat{z})\hat{p}_y \right]$$

$$= \underbrace{\hat{y}[\hat{p}_z, \hat{z}]}_{-i\hbar}\hat{p}_x - \hat{z}\underbrace{[\hat{p}_y, \hat{p}_x]}_{0}\hat{z} - \hat{p}_z\underbrace{[\hat{y}, \hat{x}]}_{0}\hat{p}_z$$

$$+ \hat{x}\underbrace{[\hat{z}, \hat{p}_z]}_{i\hbar}\hat{p}_y$$

$$= i\hbar \left\{ \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \right\} = i\hbar \hat{L}_z$$

$$\Rightarrow [\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

$\boxed{\text{A10/Q1}}$ Show that $[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$

$\boxed{\text{A10/Q2}}$ Show that $[\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$

<u>Using Index Notation</u> →

$$[\hat{L}_i, \hat{L}_j] = i\hbar\, \epsilon_{ijk} \hat{L}_k$$

→ fundamental commutation relations of angular momentum operator.

$$[\hat{L}_x, \hat{L}_y] \neq 0$$

$$\Rightarrow \hat{L}_x \hat{L}_y \neq \hat{L}_y \hat{L}_x$$

Demo:
$$R_x\left(\theta=\frac{\pi}{2}\right)R_y\left(\theta=\frac{\pi}{2}\right) \neq R_y\left(\theta=\frac{\pi}{2}\right)R_x\left(\theta=\frac{\pi}{2}\right)$$

. angular momentum operator are the generators of rotation.

(*) Wave function is translated

$$\psi(x+\Delta x) = \psi(x) + \Delta x \frac{d}{dx}\psi(x)$$
$$= \left(\mathbb{I} + \Delta x \frac{d}{dx}\right)\psi(x)$$
$$= \left(\mathbb{I} + \frac{i}{\hbar}\Delta x \frac{\hbar}{i}\frac{d}{dx}\right)\psi(x)$$

$$\Rightarrow \boxed{\psi(x+\Delta x) = \left(\mathbb{I} + \frac{i\Delta x}{\hbar}\hat{P}_x\right)\psi(x)}$$

$$\Rightarrow \boxed{\psi(x+\Delta x) = \tau(\Delta x)\,\psi(x)}$$

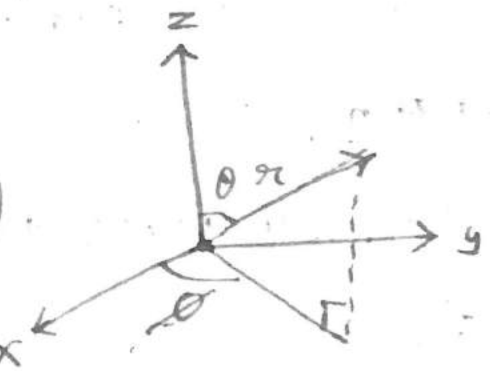
Where we have, $\boxed{\tau(\Delta x) = \mathbb{I} + i\left(\frac{\Delta x}{\hbar}\right)\hat{P}_x}$

$\tau(\Delta x)$: is a translation operator that takes a wave function at x (i.e $\psi(x)$) and returns ψ at $x+\Delta x$ (i.e $\psi(x+\Delta x)$)

$\hat{P}_x \rightarrow$ generator of the translation.

In 3D:

$$\psi(x,y,z) = \psi(r,\theta,\phi)$$



* $$\psi(r,\theta,\phi+\Delta\phi)$$

$$= \psi(r,\theta,\phi) + \Delta\phi \frac{\partial}{\partial\phi}\psi(r,\theta,\phi)$$

$$= \left[\mathbb{I} + \frac{i\,\Delta\phi}{\hbar}\left(\frac{\hbar}{i}\frac{\partial}{\partial\phi}\right)\right]\psi(r,\theta,\phi)$$

$\therefore$ $\boxed{\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}}$ in spherical polar coordinates.

$\hat{L}_z$ — is the generator of the rotation around z-axis.

* Square magnitude of the angular momentum $\vec{L}$

$$L^2 = \vec{L}\cdot\vec{L} = L_x^2 + L_y^2 + L_z^2$$

$$\Rightarrow \hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

* $$[\hat{L}^2, \hat{L}_x] = [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_x]$$

$$= [\hat{L}_x^2, \hat{L}_x] + [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x]$$

$$= \hat{L}_y[\hat{L}_y, \hat{L}_x] + [\hat{L}_y, \hat{L}_x]\hat{L}_y$$
$$+ \hat{L}_z[\hat{L}_z, \hat{L}_x] + [\hat{L}_z, \hat{L}_x]\hat{L}_z$$

$$\Rightarrow [\hat{L}^2, \hat{L}_x] = \hat{L}_y(i\hbar\hat{L}_z) + (-i\hbar\hat{L}_z)\hat{L}_y + \hat{L}_z(i\hbar\hat{L}_y) + (i\hbar\hat{L}_y)\hat{L}_z$$

$$= i\hbar[\cancel{\hat{L}_z\hat{L}_y} - \cancel{\hat{L}_z\hat{L}_y} + \cancel{\hat{L}_y\hat{L}_z} - \cancel{\hat{L}_y\hat{L}_z}]$$

$\Rightarrow \boxed{[\hat{L}^2, \hat{L}_x] = 0}$

[A10/Q3] Show that $[\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z^2] = 0$

$\rightarrow \boxed{[\hat{L}^2, \vec{\hat{L}}] = 0 \quad ; \quad \vec{\hat{L}} = \hat{i}\,\hat{L}_x + \hat{j}\,\hat{L}_y + \hat{k}\,\hat{L}_z}$

Claim: If $|\Psi\rangle$ is an eigenstate of an operator $\hat{A}$ then $|\Psi\rangle$ is also an eigenstate of the operator $\hat{B}$ if $[\hat{A}, \hat{B}] = 0$

Proof: Say $\boxed{\hat{A}|\Psi\rangle = \lambda_A |\Psi\rangle}$

$$|\Psi\rangle \xrightarrow{\hat{B}} |\Phi\rangle = \hat{B}|\Psi\rangle$$

$$A|\Phi\rangle = \hat{A}(\hat{B}|\Psi\rangle) = (\hat{A}\hat{B})|\Psi\rangle = (\hat{B}\hat{A})|\Psi\rangle$$
$$= \hat{B}(\hat{A}|\Psi\rangle) = \lambda_A \hat{B}|\Psi\rangle$$
$$= \lambda_A |\Phi\rangle$$

$\Rightarrow \boxed{\hat{A}|\Phi\rangle = \lambda_A |\Phi\rangle}$

$\Rightarrow |\Phi\rangle$ is an eigenvector of $\hat{A}$ with eigenvalue λ_A

$$\Rightarrow |\phi\rangle \propto |\Psi\rangle$$

[True only if A has no degeneracy]

$\Rightarrow |\phi\rangle = \lambda_B |\Psi\rangle$ for some $\lambda_B \in \mathbb{R}$

$\Rightarrow |\phi\rangle = \hat{B}|\Psi\rangle$

$\Rightarrow \boxed{\hat{B}|\Psi\rangle = \lambda_B |\Psi\rangle}$

⇒ If $[\hat{A}, \hat{B}] = 0$ then eigenstates of $\hat{A}$ are also the eigenstates of $\hat{B}$

Say Eigenstate of $\hat{L}^2$ are $|\psi\rangle$

$$\hat{L}^2 |\psi\rangle = \lambda |\psi\rangle$$

$$\hat{L}_z |\psi\rangle = \mu |\psi\rangle$$

as $[\hat{L}^2, \hat{L}_z] = 0$

✱ What are μ and λ?

~~Wex~~ We employ the operator method (as in SHO, $\hat{a}$, $\hat{a}^\dagger$)

Define,

$$\hat{L}_+ \equiv \hat{L}_x + i\hat{L}_y$$

$$\hat{L}_- \equiv \hat{L}_x - i\hat{L}_y$$

✱ $[\hat{L}_+, \hat{L}_-] = [\hat{L}_x + i\hat{L}_y, \hat{L}_x - i\hat{L}_y]$

$$= i[\hat{L}_y, \hat{L}_x] - i[\hat{L}_x, \hat{L}_y]$$

$$= -i\left[[\hat{L}_x, \hat{L}_y] - [\hat{L}_y, \hat{L}_x]\right]$$

$$= 2\hbar\hat{L}_z$$

$$[\hat{L}_z, \hat{L}_+] = [\hat{L}_z, \hat{L}_x] + i[\hat{L}_z, \hat{L}_y]$$
$$= i\hbar \hat{L}_y + \hbar \hat{L}_x$$
$$= \hbar(\hat{L}_x + i\hat{L}_y)$$
$$= \hbar \hat{L}_+$$
$$\Rightarrow \boxed{[\hat{L}_z, \hat{L}_+] = \hbar \hat{L}_+}$$

$$[\hat{L}_z, \hat{L}_-] = [\hat{L}_z, \hat{L}_x] - i[\hat{L}_z, \hat{L}_y]$$
$$= i\hbar \hat{L}_y - \hbar \hat{L}_x$$
$$= -\hbar(\hat{L}_x - i\hat{L}_y)$$
$$= -\hbar \hat{L}_-$$
$$\Rightarrow \boxed{[\hat{L}_z, \hat{L}_\pm] = \pm\hbar \hat{L}_\pm}$$

$$\boxed{[\hat{L}^2, \hat{L}_\pm] = 0}$$

We have,

$$\hat{L}^2|\psi\rangle = \lambda|\psi\rangle \; ; \; \hat{L}_z|\psi\rangle = \mu|\psi\rangle$$

$$\left.\begin{array}{l}[\lambda] = [\hbar^2] \\ [\mu] = [\hbar]\end{array}\right\} \Rightarrow \boxed{\begin{array}{c}\lambda = q\hbar^2 \\ \mu = m\hbar\end{array}}$$

q, m are dimensionless

By Dirac notation,

$$|\psi\rangle \Rightarrow |q, m\rangle$$

$$\hat{L}^2 |q, m\rangle = q\hbar^2 |q, m]$$

$$\hat{L}_z |q, m\rangle = m\hbar |q, m\rangle$$

o Action of $\hat{L}_{\pm}$ on $|q, m\rangle \longrightarrow$

Define,

$$|\phi\rangle := \hat{L}_{\pm} |q, m\rangle$$

$$\hat{L}_z |\phi\rangle = \hat{L}_z \hat{L}_{\pm} |q, m\rangle$$

$$= (\pm\hbar \hat{L}_{\pm} + \hat{L}_{\pm}\hat{L}_z) |q, m\rangle$$

$$= \hat{L}_{\pm} (\pm\hbar |q, m\rangle + m\hbar |q, m\rangle)$$

$$= (m \pm 1)\hbar (\hat{L}_{\pm} |q, m\rangle)$$

$$= (m \pm 1)\hbar |\phi\rangle$$

$\Rightarrow |\phi\rangle$ is an eigenvector of $\hat{L}_z$ with eigenvalue

$(m \pm 1)\hbar$

$$\Rightarrow |\phi\rangle = |q, m'\rangle$$

$$\boxed{m' = (m \pm 1)}$$

$$\boxed{\hat{L}_+ |q,m\rangle = c_1 |q, m+1\rangle}$$ Raising operator

$$\boxed{\hat{L}_- |q,m\rangle = c_2 |q, m-1\rangle}$$ Lowering operator

(7) $\hat{L}^2 - \hat{L}_z^2 = \hat{L}_x^2 + \hat{L}_y^2$

$$\langle q,m| (\hat{L}^2 - \hat{L}_z^2) |q,m\rangle = \langle q,m| (\hat{L}_x^2 + \hat{L}_y^2) |q,m\rangle$$

$$(q-m^2)\hbar^2 = \langle q,m| \hat{L}_x^2 |q,m\rangle + \langle q,m| \hat{L}_y^2 |q,m\rangle$$

Define,

$$|x\rangle = \hat{L}_x |q,m\rangle$$

$$\hat{L}_x^2 = \hat{L}_x \hat{L}_x$$

$$= \hat{L}_x^{+} \hat{L}_x$$

$$\Rightarrow \langle x|x\rangle = \langle q,m| \hat{L}_x^{+} \hat{L}_x |q,m\rangle = \langle q,m| \hat{L}_x^2 |q,m\rangle$$

$$\Rightarrow (q-m^2)\hbar^2 \geq 0$$

$$\Rightarrow \boxed{q \geq m^2}$$

For a given q, there must be a pair (m_{max}, m_{min}) such that,

$$\hat{L}_+ |q, m_{max}\rangle = 0$$

$$\hat{L}_- |q, m_{min}\rangle = 0$$

$$\hat{L}_+ \hat{L}_- = (\hat{L}_x + i\hat{L}_y)(\hat{L}_x - i\hat{L}_y)$$

$$= \hat{L}_x + \hat{L}_y^2 + i[\hat{L}_y, \hat{L}_x]$$

$$= (\hat{L}^2 - \hat{L}_z^2) + i(-i\hbar \hat{L}_z)$$

$$= \hat{L}^2 - \hat{L}_z^2 + \hbar \hat{L}_z$$

$$\Rightarrow \boxed{\hat{L}^2 = \hat{L}_+ \hat{L}_- + \hat{L}_z^2 - \hbar \hat{L}_z}$$

$$\hat{L}^2 |q, m_{min}\rangle = (\hat{L}_+ \hat{L}_- + \hat{L}_z - \hbar \hat{L}_z)|q, m_{min}\rangle$$

$$\Rightarrow q\hbar^2 |q, m_{min}\rangle = (m_{min}^2 \hbar^2 - m_{min}\hbar^2)|q, m_{min}\rangle$$

$$\Rightarrow \boxed{q = (m_{min} - 1)\, m_{min}} \longrightarrow \text{(I)}$$

Similarly,

$$\boxed{\hat{L}^2 = \hat{L}_- \hat{L}_+ + \hat{L}_z^2 + \hbar \hat{L}_z}$$

$$\hat{L}^2 |q, m_{max}\rangle = (\hat{L}_- \hat{L}_+ + \hat{L}_z^2 + \hbar \hat{L}_z)|q, m_{max}\rangle$$

$$\Rightarrow \boxed{q = m_{max}(m_{max} + 1)} \longrightarrow \text{(II)}$$

$\text{II} - \text{I} \Rightarrow m_{max}^2 - m_{min}^2 + m_{max} + m_{min} = 0$

$\Rightarrow (m_{max} + m_{min})(m_{max} - m_{min} + 1) = 0$

We Know,

$$m_{max} \geq m_{min}$$

$$\Rightarrow m_{max} = -m_{min} =: l$$

$$\Rightarrow \boxed{q = l(l+1)} \; ; \; m_{max} = l$$
$$m_{min} = -l$$

(*) m changes in steps of integers.

$\Rightarrow m_{min}, m_{min}+1, m_{min}+2, \ldots, m_{max}-2, m_{max}-1, m_{max}$

$\Rightarrow m_{max} = m_{min} + N$ for some integer N.

$$\Rightarrow 2l = N$$

$$\Rightarrow \boxed{m_{max} = l = \frac{N}{2}}$$

$$|q, m\rangle \rightarrow |l, m\rangle$$

$$\boxed{\hat{L}^2 |l,m\rangle = l(l+1)\hbar^2 |l,m\rangle}$$

$$\boxed{\hat{L}_z |l,m\rangle = m\hbar |l,m\rangle}$$

$$l = \frac{N}{2}, \quad N \in \mathbb{Z}_{\geq 0}$$

$$\Rightarrow l \in \left\{0, \frac{1}{2}, 1, \frac{3}{2}, \ldots\right\}$$

$\Rightarrow m \in \{-l, -l+1, \ldots, l-1, l\}$

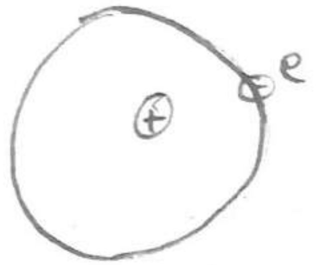
from $l(l+1) \geq m^2$

<u>Cases</u> $l = 1/2$, $m = -\frac{1}{2}, \frac{1}{2}$

$l = 1$, $m = -1, 0, 1$

$l = \frac{3}{2}$, $m = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$

Hydrogen Atom in QM



(*) Hamiltonian

$H = KE + PE$

(*) We shall assume :

$m_p \gg m_e$

(*) Potential energy (of the electron) :

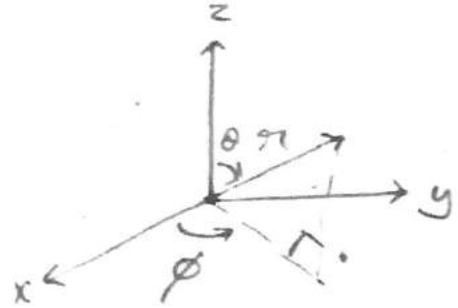
$$\boxed{V = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}}$$

(*) Kinetic Energy $= \frac{\vec{p}\cdot\vec{p}}{2m}$

where $\vec{p} = m\frac{d\vec{r}}{dt}$ in 3D

(4) Given v depends only on r, its convenient to use spherical polar coordinate

$$X = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$



Position vector :

$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$$
$$= r\hat{r}$$

$$\hat{r} = \frac{\vec{r}}{r} = \sin\theta\cos\phi\,\hat{i} + \sin\theta\sin\phi\,\hat{j} + \cos\theta\,\hat{k}$$

Momentum : $\vec{p} = m\frac{d\vec{r}}{dt}$

Cartesian : $m\left(\frac{dx}{dt}\hat{i} + x\overbrace{\frac{d\hat{i}}{dt}}^{=0} + \frac{dy}{dt}\hat{j} + y\overbrace{\frac{d\hat{j}}{dt}}^{=0} + \frac{dz}{dt}\hat{k} + z\overbrace{\frac{d\hat{k}}{dt}}^{=0}\right)$

$$\hat{p} = m\frac{d\vec{r}}{dt}$$
$$= m\left(\frac{dx}{dt}\hat{i} + \frac{dy}{dt}\hat{j} + \frac{dz}{dt}\hat{k}\right)$$

Spherical polar : $\vec{p} = m\frac{d\vec{r}}{dt} = m\left(\frac{dr}{dt}\hat{r} + r\frac{d\hat{r}}{dt}\right)$

$$= m\frac{dr}{dt}\hat{r} + r\frac{d\hat{r}}{dt}$$
$$= p_r\hat{r} + r\frac{d\hat{r}}{dt}$$

$$\boxed{\frac{\vec{p}\cdot\vec{p}}{2m} = \frac{p_r^2}{2m} + \frac{1}{2}mr^2\left(\frac{d\hat{r}}{dt}\cdot\frac{d\hat{r}}{dt}\right)} + (\quad)\overbrace{\left(\hat{r}\cdot\frac{d\hat{r}}{dt}\right)}^{=0}$$

Angular Momentum:

$$\vec{L} = \vec{r} \times \vec{p} = r\hat{r} \times \left(p_r \hat{r} + m r \frac{d\hat{r}}{dt} \right)$$

$$\Rightarrow \boxed{\vec{L} = m r^2 \left(\hat{r} \times \frac{d\hat{r}}{dt} \right)}$$

Recall:

Cartesian:

$$\hat{i} \cdot \hat{j} = \hat{j} \cdot \hat{k} = \hat{k} \cdot \hat{i} = 0$$

$$\hat{i} \times \hat{j} = \hat{k}$$

$$\hat{j} \times \hat{k} = \hat{i}$$

$$\hat{k} \times \hat{i} = \hat{j}$$

Spherical polar:

$$\hat{r} \cdot \hat{\theta} = \hat{\theta} \cdot \hat{\phi} = \hat{\phi} \cdot \hat{r} = 0$$

$$\hat{r} \times \hat{\theta} = \hat{\phi}$$

$$\hat{\theta} \times \hat{\phi} = \hat{r}$$

$$\hat{\phi} \times \hat{r} = \hat{\theta}$$

Since $\hat{r} \cdot \frac{d\hat{r}}{dt} = 0$

$$\Rightarrow \frac{d\hat{r}}{dt} = a\hat{\theta} + b\hat{\phi}$$

$$\hat{r} \times \frac{d\hat{r}}{dt} = a\hat{\phi} - b\hat{\theta}$$

$$L^2 = \vec{L}\cdot\vec{L}$$

$$= m^2 r^4 \left(\hat{r}\times\frac{d\hat{r}}{dt}\right)\cdot\left(\hat{r}\times\frac{d\hat{r}}{dt}\right)$$

$$= m^2 r^2 (a^2 + b^2)$$

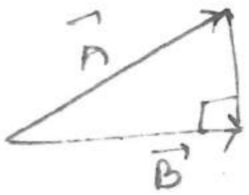
$$= m^2 r^2 \left(\frac{d\hat{r}}{dt}\right)\cdot\left(\frac{d\hat{r}}{dt}\right)$$

$$\frac{p^2}{2m} = \frac{p_r^2}{2m} + \frac{1}{2} m r^2 \left(\frac{d\hat{r}}{dt}\cdot\frac{d\hat{r}}{dt}\right)$$

$$= \frac{p_r^2}{2m} + \frac{1}{2mr^2} L^2$$

$$\Rightarrow \boxed{KE = \frac{p^2}{2m} = \frac{1}{2m}\left(p_r^2 + \frac{L^2}{r^2}\right)}$$

Let $\vec{A}$ be a given vector and $\hat{B}$ be unit vector such that $\hat{A} \neq \hat{B}$



$$\vec{A} = \vec{B} + \vec{C}$$

$$\Rightarrow \vec{A}\cdot\vec{A} = \vec{B}\cdot\vec{B} + \vec{C}\cdot\vec{C}$$

$$\Rightarrow \vec{A}\cdot\vec{A} = \cancel{\vec{B}}\,(\hat{B}\cdot\vec{A})^2 + (\hat{B}\times\vec{A})^2$$

Set $\hat{B} = \hat{r}$ and $\vec{A} = \vec{p}$

$$\Rightarrow \vec{p}\cdot\vec{p} = (\hat{r}\cdot\vec{p})^2 + \cancel{\vec{m}}\,(\hat{r}\times\vec{p})^2$$

$$\Rightarrow p^2 = p_r^2 + \left(\frac{\vec{r}\times\vec{p}}{r}\right)^2$$

$$\Rightarrow \boxed{p^2 = p_r^2 + \frac{L^2}{r^2}}$$

o <u>Time-independent Schrodinger Eqn:</u>

$$\hat{H}\Psi = E\Psi \quad \Big| \quad \Psi = \Psi(r,\theta,\phi)$$

Classically,

$$H = KE + V$$

$$\Rightarrow \hat{H}\Psi = \left[\frac{\hat{p}_r^2}{2m} + \frac{1}{2mr^2}\hat{L}^2 + V(r)\right]\Psi$$

$$= E.\Psi$$

(*) What are these $|l, m\rangle$ ket states in (θ, ϕ) representation?

<u>Recall SHO</u>.

Ground state: $|0\rangle$

We have seen $\psi_0(x) = \langle x|0\rangle$
$$= \mathcal{N} e^{-\alpha x^2}$$

$$\psi_1(x) = \langle x|1\rangle = \mathcal{N} x e^{-\alpha x^2}$$

In general,

$$\boxed{\psi_n(x) = \langle x|n\rangle = \mathcal{N} H_n(\beta x) e^{-\alpha x^2}}$$

α, β are appropriate const.

where $H_n(x) \rightarrow$ Hermite polynomials.

$H_0(x) = 1$

$H_1(x) = 2x$

$H_2(x) = 4x^2 - 2$

$H_n(x) = e^{x^2}\left(\frac{d}{dx}\right)^n e^{-x^2}$

(*) Similarly,

$$\boxed{\Psi_{l,m}(\theta, \phi) = \langle \theta, \phi | l, m \rangle \equiv Y_{lm}(\theta, \phi)}$$

$\hookrightarrow$ Spherical Harmonics.

$$\Rightarrow \begin{cases} \hat{L}^2 |l, m\rangle = l(l+1)\hbar^2 |l, m\rangle \\ \hat{L}_z |l, m\rangle = m\hbar |l, m\rangle \end{cases}$$

$$\rightarrow \hat{L}^2 Y_{lm}(\theta, \phi) = l(l+1)\hbar^2 Y_{lm}(\theta, \phi)$$

$$\rightarrow \hat{H}\Psi = \left[\frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} + \hat{V}(r)\right]\Psi = E\Psi$$

Here, $\Psi = \Psi(r, \theta, \phi) = R(r)\, Y_{lm}(\theta, \phi)$ (Ansatz)

$\Rightarrow$ <u>Radial wave function</u> $(R = R(r))$

$$\boxed{\hat{p}_r^2 R(r) + \left[2m\left(\hat{V}(r) - E\right) + \frac{l(l+1)\hbar^2}{r^2}\right] R(r) = 0}$$

(*) What is the operator $\hat{p}_r$?

Classically, $p_r = \frac{1}{r}(\vec{r} \cdot \vec{p})$

$= \frac{1}{r}(x p_x + y p_y + z p_z)$

Say, $\hat{P}_r = \frac{1}{r}(\hat{x}\hat{p}_x + \hat{y}\hat{p}_y + \hat{z}\hat{p}_z)$

$\hat{P}_r^{+} \neq \hat{P}_r$ as $\vec{r}$ and $\vec{p}$ are non-commuting operators.

⊛ How do we make $\hat{p}_r$ Hermitian ?

We can choose

$$\boxed{\hat{P}_r = \frac{1}{2}\left(\frac{\hat{\vec{r}}}{r}\cdot\hat{\vec{p}} + \hat{\vec{p}}\cdot\frac{\hat{\vec{r}}}{r}\right)}$$

⊛ Operator form of $\frac{\hat{\vec{r}}}{r}\cdot\hat{\vec{p}}$ [in polar coordinates]

$$\hat{\vec{p}} = \frac{\hbar}{i}\vec{\nabla} = \frac{\hbar}{i}\left(\hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}\right)$$

Say, $\frac{\hat{\vec{r}}}{r}\cdot\hat{\vec{p}}\,\psi = \frac{\hbar}{i}\frac{1}{r}\left(x\frac{\partial\psi}{\partial x} + y\frac{\partial\psi}{\partial y} + z\frac{\partial\psi}{\partial z}\right)$

Since $\psi = \psi(r)$

$$\frac{\partial\psi}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial\psi}{\partial r} = \left(\frac{x}{r}\right)\frac{\partial\psi}{\partial r}$$

$$\frac{\hat{\vec{r}}}{r}\cdot\hat{\vec{p}}\,\psi = \frac{\hbar}{i}\left(\frac{x^2}{r^2}\frac{\partial\psi}{\partial r} + \frac{y^2}{r^2}\frac{\partial\psi}{\partial r} + \frac{z^2}{r^2}\frac{\partial\psi}{\partial r}\right)$$

$$\Rightarrow \boxed{\frac{\hat{\vec{r}}}{r}\cdot\hat{\vec{p}}\,\psi = \left(\frac{\hbar}{i}\frac{\partial}{\partial r}\right)\psi}$$

$$\Rightarrow \boxed{\frac{\hat{\vec{r}}}{r}\cdot\hat{\vec{p}} = \hat{r}\cdot\hat{\vec{p}} = \frac{\hbar}{i}\frac{\partial}{\partial r}}$$

$$\hat{p}_r \psi = \frac{1}{2}\frac{\hbar}{i}\left[\frac{\vec{r}}{r}\cdot\vec{\nabla}\psi + \vec{\nabla}\left(\frac{\vec{r}}{r}\psi\right)\right]$$

$$= \frac{1}{2}\frac{\hbar}{i}\left[\frac{\vec{r}}{r}\vec{\nabla}\psi + \psi\vec{\nabla}\left(\frac{\vec{r}}{r}\right) + \frac{\vec{r}}{r}\vec{\nabla}\psi\right]$$

$$= \frac{1}{2}\frac{\hbar}{i}\left[2\frac{\vec{r}}{r}\vec{\nabla}\psi + \psi\vec{\nabla}\left(\frac{\vec{r}}{r}\right)\right]$$

$$\vec{\nabla}\cdot\left(\frac{\vec{r}}{r}\right) = \frac{1}{r}\left(\vec{\nabla}\cdot\vec{r}\right) + \vec{r}\left(\vec{\nabla}\cdot\left(\frac{1}{r}\right)\right)$$

$$= \frac{3}{r} + \vec{r}\cdot\left\{\frac{\partial}{\partial x}\left(\frac{1}{r}\right)\hat{i} + \frac{\partial}{\partial y}\left(\frac{1}{r}\right)\hat{j} + \frac{\partial}{\partial z}\left(\frac{1}{r}\right)\hat{k}\right\}$$

$$= \frac{3}{r} + \left[-\frac{\vec{r}}{r^2}\cdot\left\{\frac{x}{r}\hat{i} + \frac{y}{r}\hat{j} + \frac{z}{r}\hat{k}\right\}\right]$$

$$= \frac{3}{r} + \left(-\frac{(x^2+y^2+z^2)}{r^3}\right)$$

$$= \frac{2}{r}$$

$$\Rightarrow \hat{P}_r\psi = \frac{\hbar}{i}\left[\frac{\vec{r}}{r}\vec{\nabla}\cdot\psi + \frac{1}{r}\psi\right]$$

$$= \frac{\hbar}{i}\left[\frac{\partial}{\partial r}\psi + \frac{1}{r}\psi\right] \Rightarrow \frac{\hbar}{i}\left[\frac{1}{r} + \frac{\partial}{\partial r}\right]\psi$$

$$= \frac{\hbar}{i}\left[\frac{1}{r}\frac{\partial}{\partial r}r\right]\psi$$

(*) <u>Radial wave function $R(r)$</u>

$$\hat{P}_r R(r) = \left[2m\left(V(r) - E\right) + \frac{\hbar^2(l)(l+1)}{r^2}\right]R(r) = 0$$

$\rightarrow$ we define $u(r) = rR(r)$

$$\hat{P}_r R(r) = \frac{\hbar}{i}\frac{1}{r}\frac{d}{dr}\left(rR(r)\right) = \frac{\hbar}{i}\frac{1}{r}\frac{d}{dr}u(r)$$

$$\hat{P}_r^2 R(r) = \hat{P}_r\hat{P}_r R(r)$$

$$= \frac{\hbar}{i}\frac{1}{r}\frac{d}{dr}\left[\cancel{r}\frac{\hbar}{i}\frac{1}{\cancel{r}}\frac{d}{dr}u(r)\right]$$

$$= -\frac{\hbar^2}{r}\frac{d^2}{dr^2}u(r)$$

$$\Rightarrow \boxed{-\frac{\hbar^2}{r}\frac{d^2}{dr^2}u(r) + \left[2m\left(V(r)-E\right) + \frac{\hbar^2 l(l+1)}{r^2}\right]u(r) = 0}$$

— (*)

Say $k^2 = -\frac{2mE}{\hbar^2}$ | $E<0$

$$\frac{d^2}{dr^2}u - \left[-\frac{2m}{\hbar^2}\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r} + k^2 + \frac{l(l+1)}{r^2}\right]u(r) = 0$$

(*) We define $\boxed{\rho = kr}$ $\quad [k] = \frac{1}{[L]}$

Now divide by k^2 in eqn.

$$\frac{d^2u}{d\rho^2} - \left[1 - \frac{me^2}{2\pi\varepsilon_0\hbar^2 k}\frac{1}{\rho} + \frac{l(l+1)}{\rho^2}\right]u = 0$$

↳ ρ_0 (define)

ρ is unitless

$$\boxed{\frac{d^2u}{d\rho^2} - \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right]u = 0} \quad \text{— (*)(*)}$$

→ A ~~net~~ neat form of the Schroedinger eqn for radial wave function.

(*) Asymptotics Solutions.

[I] for large $r \Rightarrow$ large ρ

for $\rho >> 1$

$$\boxed{\frac{d^2u}{d\rho^2} - u = 0} \Rightarrow u = Ae^{-\rho} + Be^{-\rho}$$

for $r \to \infty$, $R(r) < \infty \Rightarrow B = 0$

$$\Rightarrow \boxed{R(r) = \frac{1}{r} A e^{-Rr}}$$

$\boxed{\text{II}}$ For small r (i.e. small ρ)

$$\Rightarrow \frac{d^2u}{d\rho^2} - \frac{l(l+1)}{\rho^2} u = 0$$

Claim : The general solution : $u = C\rho^{l+1} + D\rho^{-l}$

Proof : $\frac{du}{d\rho} = (l+1)C\rho^{l} - Dl\rho^{-(l+1)}$

$$\frac{d^2u}{d\rho^2} = l(l+1)C\rho^{l-1} + Dl(l+1)\rho^{-(l+2)}$$

$$\Rightarrow l(l+1)C\rho^{l-1} + l(l+1)\rho^{-(l+2)}$$

$$= l(l+1)\left[C\rho^{l-1} + D\rho^{-(l+2)}\right]$$

$$= \frac{l(l+1)}{\rho^2}\left[C\rho^{l+1} + D\rho^{-l}\right]$$

$$= \frac{l(l+1)}{\rho^2} u$$

$$= \frac{d^2u}{d\rho^2} - \frac{l(l+1)}{\rho^2} u = 0$$

$$R(r) = \frac{1}{r}\left(C(Rr)^{l+1} + D(Rr)^{-l}\right)$$

for $R(r) < \infty$ for $r \to 0 \Rightarrow D = 0$

$$\boxed{R(r) \sim r^{l}}$$

In summary:

$$\rho \to \infty ; \quad u = A e^{-\rho}$$

$$\rho \to 0 ; \quad u = C \rho^{l+1}$$

Ansatz: $\boxed{u = \rho^{l+1} e^{-\rho} v(\rho)}$

$$\frac{du}{d\rho} = (l+1)\rho^{l} e^{-\rho} v - \rho^{l+1} e^{-\rho} v + \rho^{l+1} e^{-\rho} \frac{dv}{d\rho}.$$

$$\begin{aligned}\frac{d^2u}{d\rho^2} = {} & l(l+1)\rho^{l-1} e^{-\rho} v - (l+1)\rho^{l} e^{-\rho} v \\ & + (l+1)\rho^{l} e^{-\rho} \frac{dv}{d\rho} \\ & - (l+1)\rho^{l} e^{-\rho} v + \rho^{l+1} e^{-\rho} v - \\ & \rho^{l+1} e^{-\rho} \frac{dv}{d\rho} \\ & + (l+1)\rho^{l} e^{-\rho} \frac{dv}{d\rho} - \rho^{l+1} e^{-\rho} \frac{dv}{d\rho} \\ & + \rho^{l+1} e^{-\rho} \frac{d^2v}{d\rho^2}\end{aligned}$$

$$\begin{aligned}\Rightarrow & \left[1 - \frac{2(l+1)}{\rho} + \frac{l(l+1)}{\rho^2}\right] \rho^{l+1} e^{-\rho} v \\ & - 2\left[1 - \frac{(l+1)}{\rho}\right] \rho^{l+1} e^{-\rho} \frac{dv}{d\rho} \\ & + \rho^{l+1} e^{-\rho} \frac{d^2 v}{d\rho^2}\end{aligned}$$

We Know,

$$\frac{d^2 v}{d\rho^2} - \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right] u = 0$$

$$\Rightarrow \boxed{\frac{d^2 v}{d\rho^2} - 2\left[1 - \frac{(l+1)}{\rho}\right] \frac{dv}{d\rho} - \left[\frac{2(l+1) - \rho_0}{\rho}\right] v = 0}$$

Let's define,

$$x = 2\rho$$

$$y(x) = \vartheta(\rho)$$

$$\alpha = 2l+1 \;;\; \beta = \frac{1}{2}\left[\rho_0 - 2(l+1)\right]$$

$$\Rightarrow 4\frac{d^2y}{dx^2} - 4\left(1 - \frac{\alpha+1}{x}\right)\frac{dy}{dx} + \frac{4\beta}{x}y = 0$$

$$\Rightarrow \boxed{xy'' + (\alpha+1-x)y' + \beta y = 0}$$

↳ Associated Laguerre differential eqn

(*) It has exact solution which lead to normalizable radial wave function $(rR(r))$ provided β is a non-negative integer

$[\text{i.e., } \beta = N = 0, 1, 2, 3, \ldots]$

These solution are known as the associated Laguerre Polynomial and denoted as,

$$L_N^{\alpha}(x) = y(x) = \vartheta(\rho)$$

$$L_0^{\alpha}(x) := 1$$

$$L_1^{\alpha}(x) := 1 + \alpha - x \ldots$$

Condition of ρ and l

$$\beta = \frac{1}{2}\left[\rho_0 - 2(l+1)\right] = N \geq 0$$

$$\Rightarrow 2(l+1) \leq \rho_0 \quad \text{as } N \geq 0$$

$$\Rightarrow \boxed{\rho_0 = 2(N + l + 1)}$$

We Know,

$$l = \frac{N}{2}$$

$$l \in \left\{0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots\right\}$$

Case (I) : $l = 0, 1, 2, \dots$

$$\rho_0 = 2[N + l + 1] = 2n$$

Where $\boxed{n = N + l + 1 = 1, 2, 3, \dots}$

$$\Rightarrow l + 1 \leq \frac{\rho_0}{2} = n$$

$$\Rightarrow l \leq n - 1$$

$$\Rightarrow \boxed{l = 0, 1, \dots, n-1}$$

$$\rho_0 = \frac{me^2}{2\epsilon_0 \hbar^2 \pi R}$$

* Energy eigen values :

$$E = -\frac{\hbar^2}{2m} R^2 \Rightarrow E = -\frac{\hbar^2}{2m} \frac{m^2 e^4}{4\epsilon_0^2 \pi^2 \hbar^4 \rho_0^2}$$

$$\Rightarrow E = \frac{-me^4}{8\epsilon_0^2 \pi^2 \hbar^2} \cdot \frac{1}{2^2 n^2}$$

$$\Rightarrow \boxed{E_n = -\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{1}{n^2}}$$

Bohr formula for energy levels of H atom.

Where are $l = \frac{1}{2}, \frac{3}{2}, \cdots$ eigen values or

Why $l = 0, 1, 2, \cdots$ only ?

$\hat{L}_z |l, m\rangle = m\hbar |l, m\rangle$

* $\langle \phi | \hat{L}_z | l, m\rangle = m\hbar \langle \phi | l, m\rangle$

$= \frac{\hbar}{i} \frac{\partial}{\partial \phi} \langle \phi | l, m\rangle$

Define $\langle \phi | l, m\rangle = \psi_{lm}(\phi)$

$\therefore m\hbar \psi_{lm}(\phi) = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \psi_{lm}(\phi)$

$$\Rightarrow \boxed{\psi_{lm}(\phi) = e^{im\phi} \cdot f_{lm}(\theta)}$$

$$\psi_{lm}(\phi) = \psi_{lm}(\phi + 2\pi)$$

* If we demand that the wave function be single valued function of the coordinate ϕ.

$$e^{im\phi} = e^{im(\phi + 2\pi)}$$

$$\Rightarrow e^{i2m\pi} = 1 \Rightarrow \boxed{m \in \mathbb{Z}}$$

Since $m \in \{-l, -l+1, \cdots, l-1, l\}$

l should be integer for orbital angular momentum (Not half integer).

$$\boxed{\hat{L}^2 |l, m\rangle = l(l+1)\hbar^2 |l, m\rangle} \text{ with } l = 0, 1, 2, \cdots$$

$\hookrightarrow$ orbital angular momentum operator.

(*) $l = \frac{1}{2}, \frac{3}{2}, \ldots$ → corresponds to spin angular momentum.

○ Radial wave function

$$\boxed{R(r) = \frac{1}{r}u = \frac{1}{r}\rho^{l+1}e^{-\rho}L_{\beta}^{\alpha}}$$

$\beta = \frac{1}{2}[\rho_0 - 2(l+1)]$

$\alpha = 2l+1$

$l \sim n$

$\rho_0 \sim n$ $\boxed{\alpha \sim n}$

$\boxed{\beta \sim n}$

$$\boxed{R_{nl}(r)}$$

(*) Energy eigenkets:

$$\boxed{\Psi = \Psi(r, \theta, \phi) = R_{nl}(r)\, Y_{lm}(\theta, \phi) = \Psi_{nlm}(r, \theta, \phi)}$$

In Dirac notation,

$$\boxed{\hat{H}|n, l, m\rangle = E_n|n, l, m\rangle}$$

(*) Ground state (n = 1)

$l = 0, 1, \ldots, n-1 \Rightarrow \boxed{l = 0} \Rightarrow \boxed{m = 0}$

$\hat{H}|1, 0, 0\rangle = E_1|1, 0, 0\rangle \Rightarrow \cancel{\hat{H}\,\Psi_{lm}}$

$\Rightarrow \hat{H}\,\Psi_{100} = E_1\,\Psi_{100}$

(*) First excited state $(n=2) \rightarrow l = 0, 1$

(i) $l=0, \; m=0$

$$\hat{H}\,|2,0,0\rangle = E_2\,|2,0,0\rangle$$

(ii) $l=1 \Rightarrow m=-1, 0, 1$

(a) $\hat{H}\,|2,1,-1\rangle = E_2\,|2,1,-1\rangle$

(b) $\hat{H}\,|2,1,0\rangle = E_2\,|2,1,0\rangle$

(c) $\hat{H}\,|2,1,1\rangle = E_2\,|2,1,1\rangle$

→ There is '1' state with energy E_1

→ There ~~is~~ are '4' state with energy E_2

→ ~~E~~ First excited eigenstate has 4 fold degeneracy {Same eigenvalue but different states}

n: Principal quantum no.

l: Azimuthal quantum no..

m: magnetic quantum no.