

16/10/2023

Write out the inadequacies of classical mechanics that leads to quantum mechanics.

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Answer,

Classical mechanics, while incredibly successful in explaining macroscopic phenomena, faced inadequacies when dealing with microscopic scales and high speeds. These limitations ultimately led to the development of quantum mechanics.

1 Failure at the quantum level.

Classical mechanics fails to explain phenomena at the atomic and sub-atomic levels such as the behavior of electrons within atoms, where discrete energy levels and quantized behaviors are observed.

2 Wave-particle duality

Classical mechanics could not account for the dual nature of particles which exhibits both wave-like and particle-like properties. The wave-particle duality became evident in experiments like the double-slit experiment.

Challenging classical ideas of particle behavior.

3. Uncertainty principle :- Classical mechanics assumed precise measurement was possible yet the Heisenberg uncertainty principle revealed that it's impossible to simultaneously measure certain pairs of properties like position and momentum with absolute accuracy.

#### 4. Quantization of energy

Classical mechanics did not account for the quantization of energy levels observed in phenomena like black body radiation, and the photoelectric effect where energy is discrete units or quanta.

#### 5. Need for statistical interpretation

Classical mechanics struggled with explaining statistical behavior observed in systems of many particles which became foundational in quantum mechanics with the development of statistical mechanics.

These limitations prompted the development of quantum mechanics, a theory that revolutionized our understanding of the microscopic world by introducing probabilistic descriptions wave functions and a fundamentally different set of principles governing the behavior of particles at the quantum scale.

## Annihilation of Electrons.

Electron annihilation refers to a process where an electron and its antimatter counterpart, a positron, collide and cease to exist, transforming their mass into energy.

When they annihilate, they release photons (gamma rays) with energies equivalent to the mass of the annihilating particles, following Einstein's famous equation,  $E = mc^2$ . This process conserves both energy and momentum.

The resulting gamma-ray ~~particles~~ carry the energy previously held in the mass of the electron and positron. This phenomena is crucial in various fields, including particle physics, astrophysics (such as in the interactions of cosmic rays) and medical imaging techniques (like PET scans, where positron emission is used to produce images of internal body structures).

In simpler terms,

Electron annihilation means when an electron and its opposite, a positron meet, they disappear and what is left is energy in the form of light. It is like when you have an equation where you start with two things on one side and they turn into something different on the other side. In this case, the electron and positron

Combine, and the result is energy specifically light called  
gamma rays. This process is called ANNIHILATION, <sup>and</sup> it happens  
according to Einstein's famous equation where mass can  
change into energy

$$E = \underline{mc^2}$$

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## A Inadequacies of Classical mechanics and the birth of quantum mechanics

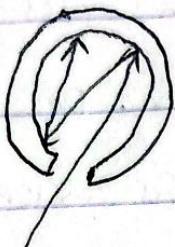
Up to the late 19th Century, the law of Physics was based on Classical (Newtonian) mechanics and Maxwell's equations for electricity and magnetism. These classical laws were early thought to be sufficient for describing all physical phenomena; however, as new physical phenomena at the atomic and sub-atomic emerged in the late 19th and early 20th Century, these laws became consistently unsatisfactory in proving satisfactory physical explanation to the newly emerging phenomena. This inadequacy lead to the development of quantum mechanics. Reasons →

- i. Black body radiation
- ii. Photoelectric emission
- iii. Atomic Spectra
- iv. Compton effect
- v. Specific heat capacity of solid

Max Planck (1858-1947)

## 1. Black body radiation

A black body is an ideal system that absorbs all radiation that incident on it. The electromagnetic radiations emitted by a black body is called black body radiation.



It depends on the temperature of the cavity.

Characteristics of the system depends on the temperature of the body. At room temperature, the wavelength of the thermal radiation are mainly in the infrared region. However, as the surface temperature increases, the wavelength changes. The object glow red, <sup>yellow</sup> orange and blue.

Light is EM wave that is produced when an electric charge vibrates.

In a hot Object, electrons vibrates in random motion as a result, light is produce. A hot object means more energy vibration and so more light is emitted as it glows <sup>larger</sup> ~~brighter~~.

Classical physics predicted that each frequency of vibration should have the same energy

Experimental result show that the black body spectrum always become short wavelength (high frequency)

In 1900, Planck proposed that each frequency of vibration should have the same energy. Instead he suggested that energy is not shared equally with electrons that vibrate. Planck explained that energy comes in packets called quanta.

<sup>Boltzmann</sup>  
Stephan - Boltzmann law : the total power of the emitted radiation increases with temperature. Joseph Stefan formulated a law which states that the radiant energy of a black body is proportional to the fourth power of its temperature.

$$J = \sigma T^4$$

Stefan's law was one of the ~~first~~ first important steps towards

The same law was theoretically derived by Ludwig Boltzmann

\* Wilhelm Wien's displacement law

He used theory about heat and electromagnetism to detect the Wien's displacement when calculates the

emission of a black body at any temperature from the emission at any w

Wien's displacement law states that black body radiation curve for different temperature peaks at the wavelength inversely proportional to the temperature

$$\lambda = \frac{B}{T}$$

$$\lambda T = B$$

$$\lambda_{\max} T = 2.898 \times 10^{-3} \text{ m K}$$

The intensity of a black body radiation increases with increasing temperature.

Rayleigh - Jean's law :- he derived a dependence  $\lambda^{-4}$ . It reveal an important error in physics theory at that time the law predicted an energy output that diverted toward infinity as wavelength approaches zero ( $F \rightarrow \infty$ ).

however, measurement of energy at short wavelength disagreed with the rayleigh - jean's law. It is given by,

$$I(\lambda, T) = \frac{2\pi c k_B T}{\lambda^4}$$

Max Planck explanation of black body radiation

Classical physics predicted that all object will instantly radiate all their heat into E.M.F. Experiments showed that the radiation rate went to infinity as E.M.F approaches zero, and it is called the UV ~~catastrophe~~ Catastrophe. Max Planck solved problem by <sup>postulation</sup> saying that E.M energy was emitted in quanta with h<sub>s</sub>

Two major assumptions

a) energy of all oscillators can have only discrete value

$$E = nhf \quad n = 1, 2, 3, 4 \quad n = \text{quantum no}$$

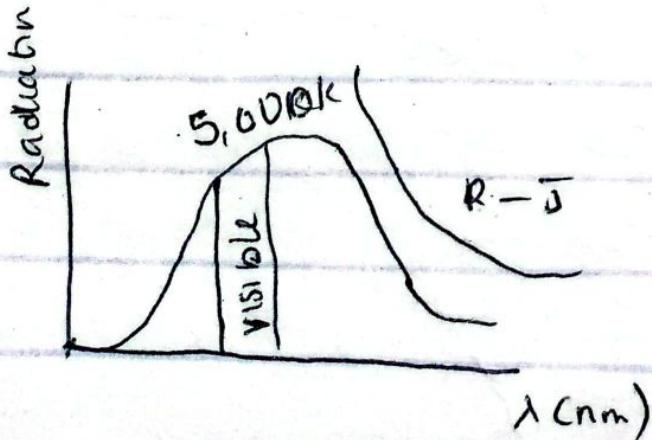
b) oscillators emit or absorb energy when making a transition from one quantum state to another.

$$\epsilon_2 - \epsilon_1 = nhf_2 - nhf_1$$

Planck's distribution function

UV catastrophe solution

$$I(\lambda, T) = \frac{2\pi hc^2}{\lambda^5} \cdot \frac{1}{(e^{\frac{hc}{\lambda kT}} - 1)}$$



### Class-work

Compute the black body radiation Intensity using the Planck's radiation distribution formulae at varying wavelength (100 - 2500 nm) for three set of temperature ( $T$ ) . 4000 K, 6000 K, 7000 K.

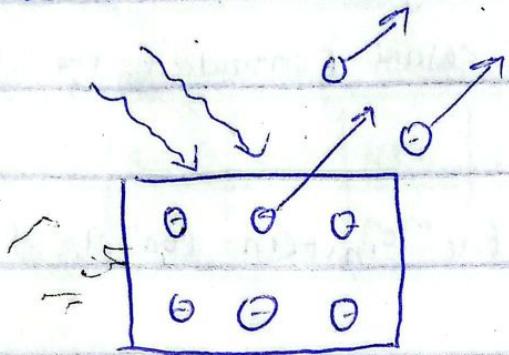
- b) Plot on a composite axis for the Planck radiation Intensity against wavelength for temperature 4000K, 6000K and 7000K. Hold the Composite axis, and plot the Rayleigh-Jean's radiation against wavelength for 7000K.
- c) Comment on the Rayleigh-Jean's radiation Intensity Curve and Planck radiation Intensity Curve:

What is the position of the peaks of the radiation intensity with respect to the origin of the wavelength axis, 4000K, 6000K and 7000K?

Estimate the order of increment in the radiation Intensity peaks for 4000K, 6000K, 7000K

## PHOTOELECTRIC EFFECT

It occurs when light is incident on a metal surface causing electrons to be emitted from such surface. The emitted electrons are called photo-electrons.



The light coming must be equal and greater than the Surface Frequency.

Frequency.

\* Classical ~~experimentation~~ and quantum experimentation.

Classical mechanics predicted that the K.E of photons depends on light intensity. As d light intensity incident on a metal is increased, electrons expected to be ejected with more energy. But experimentation shows that the ~~max~~ maximum K.E is independent of light energy but proportional to the stopping potential. The Max K.E increases with increase in light freq.

further more, electrons are expected to be ejected at any frequency as long as light intensity is high enough. However, experimental result shows that electrons are emitted if freq is below the cut off freq. The cut off frequency is a characteristic

of photo electric material to electron is emitted below the cut off freq.

At low intensities measurable time interval should pass b/w the instant, d light is turned on.

The experimental result contradict the Classical mechanics prediction.

This necessitated the Einstein concept of quantization to Electromagnet waves

$$K \cdot \epsilon (S) \rightarrow r (\text{Hz})$$

$$E = hf$$

$$K \cdot \epsilon = hf - \phi \rightarrow \begin{matrix} \gamma \text{ kinetic} \\ \text{work function} \end{matrix}$$

Klopfenfunktion  $\phi$  of metals

Metal  $\phi$  ev

Sodium 2.46

Al 4.18

Fe 4.50

Cu 4.10

Zn 4.31

Ag 4.73

Pt 6.75

Pb 4.14

We know the plot of  $k.E$  vs  $f$  is always linear

### Assignment

A Certain photo electric surface was illuminated with light of different wavelength. And the following Stopping potential are as follows

$\lambda_m$	336	405	436	492	516	579
Stopping potential (eV)	1.48	1.15	0.93	0.62	0.36	0.24

Plot a graph of  $f$  against  $eV$  and  $\lambda$

1. threshold frequency and wavelength
2. The workfunction of the material
3. The value of the Planck Constant
4. Comment on your result when the intensity of the light is assumed to be increased by a factor of 4.

## Compton Effect

### The wavelength

In 1923, Compton reported the result of his experiment on Scattering of monochromatic hard X-ray from graphite target. The wave length of the scattered radiation experiment was measured using a Bragg's Spectrometer. The Scattered radiation at a given scattered angle was passed through the Collimator.

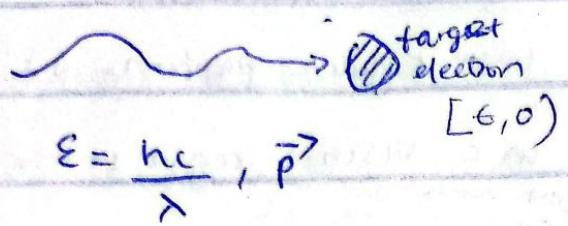
### Failure of Classical mechanics

According to the classical theory of Scattering of electromagnetic radiation from electrons, the oscillating field of the incident X-ray acts on the electrons that are contain in the atom of the target material. This interaction forces the electrons to oscillate with same freq as the incident radiation. The oscillating electrons in turn radiate E.M wave of the same frequency.

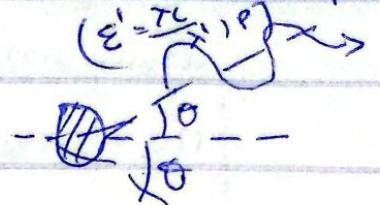
Therefore, the classical Scattering theory predicted that the wavelength of the scattered radiation must be exactly the same as that of incident radiation. Thus, it fails to explain the change in wavelength observed in Compton scattering.

As Compton Scattering is elastic or Coherence scattering in incident photon to electrons.

Before Incident photon



After Incident photon



$[E_r, P_r]$

$$\Delta h = h - h' = \frac{\lambda}{mc} (1 - \cos\theta)$$

### Atomic theory

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After Rutherford found that repulsive charge in atoms is in a thin nucleus - classical mechanics predicted that the electrons  $\Rightarrow$  orbiting  $\oplus$  nucleus would radiate their energy away and spiral into the nucleus. Certainly, this did not happen.

$$\text{Rydberg formula: } \frac{1}{\lambda} = R \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

hydrogen is used to provide the explanation, being the simplest atom has only one electron. Thus it was the simplest spectral.

The spectrum decreases in a regular pattern. Balmer showed that to the line in a visible region in the spectrum have wavelength  $\lambda = \text{Balmer series}$   $656\text{nm}, 434\text{nm}, 410\text{nm}$ .

for  $n=1$ , it produce Lyman series of line,  $\lambda = 91\text{nm} - 122\text{nm}$  and it is the ultra-violet region

for  $n=3$ , it produce the Paschen series of line of wavelength of region Infra-red

MB:- In all the series,  $n=2$  must start at

$$\text{i.e } n_2 = n_1 + 1$$

Bohrs action.

In 1913, electron orbit the nucleus like planet orbiting the sun. He postulate the hydrogen atom ( $Z=1$ ).



A typical Bohr's model

$$F_c = \frac{mv^2}{r} ; F_e = \frac{1}{4\pi\epsilon_0} \frac{ze^2}{r^2} \rightarrow \text{Centrifugal force} = \text{Electrostatic force}$$

$$f_c = f_e$$

$$\frac{mv^2}{r} = \frac{ze^2}{4\pi\epsilon_0 r^2} ; k =$$

$$L = mvr = nh$$

$$\therefore \frac{1}{r} = \frac{mZe^2}{4\pi\epsilon_0 h^2} \cdot \frac{1}{n^2}$$

$$\therefore r_n = \frac{n^2 h^2 \epsilon_0}{4\pi m Z e^2} = \frac{n^2}{1}$$

$$r_1 = \frac{h^2 \epsilon_0}{4\pi m c^2} = \text{Bohr's radius.}$$

$$r_1 = 0.529 \text{ Å}$$

$$\text{The potential energy } U = -eV = -\frac{1}{4\pi\epsilon_0} \frac{ze^2}{r}$$

The total energy of an electron in n orbit is the sum of PE and KE

$$T.E (E_n) = \frac{1}{2}mv^2 + \frac{1}{4\pi\epsilon_0} \frac{ze^2}{r_n}$$

$$E_n = -\left(\frac{z^2 e^2 m}{8\pi\epsilon_0^2 h^2}\right)\left(\frac{1}{n^2}\right) \quad n=1, 2, 3, \dots$$

$$E_n = (-13.6 \text{ eV})\left(\frac{z^2}{n^2}\right)$$

When  $A=1$  and  $z=1$ ,  $E_1 = -13.6 \text{ eV} \rightarrow$  lowest energy level.

<sup>Hydrogen</sup>  
Construct energy level diagram for  $\text{He}^{2+}$  and  $n=1, 10$ , comment on the proximity as  $n$  increase.

b) Validate the failure of Bohr's ~~SH~~ theory to Uncertainty principle  
take  $r_a = 5.3 \times 10^{-11} \text{ m}$ , electron velocity  $= 2.2 \times 10^6 \text{ m s}^{-1}$ ,  $m_e = 9.11 \times 10^{-31} \text{ kg}$   
Assuming 10% of uncertainty is associated with velocity

### Failures of Bohr Model

- It fails to explain why certain spectral lines are brighter than others - and there is no mechanism for the calculation of transition probability

2. The Bohr model treat the electrons as if it were a miniature planet with definite radius and momentum. This, which state that "position and momentum can not be simultaneously determine"  
Uncertainty principle

### Specific Heat Capacity

With classical mechanics prediction, the molar heat capacity at constant volume =  $3R$  where  $R$  = the molar gas constant.  
=  $8.314 \text{ J/Kmol}$ .

In thermodynamics, the ~~energy~~ average  $K \cdot \Sigma$  per atom in each degree of freedom  $\rightarrow \frac{1}{2} kT$   
i.e  $K \cdot \Sigma = \frac{1}{2} kT$

An atom

Wave particle duality

light can behave like a wave and like a particle.

diffraction experiment  $\rightarrow$  a wave



photoelectric effect  $\rightarrow$  a particle



Louis de Broglie (1892-1987) he postulated that light have both wave and particles characteristics. Matter also have wave property.

he assumed  $E = hf$  for photons and other particles.

He used Lorentz invariance to derived the wavelength for particles the de Broglie wavelength

$$\lambda = \frac{h}{P(mv)} \quad \text{--- (1)}$$

$\frac{h}{mv}$  λ and F  
wave like property

In term of freq, he postulate that  $f = \frac{E}{h} \quad \text{--- (2)}$  Wave &  
Particle-like  
property

from eqn 1 and 2 we can have the dual nature of matter  
Condition

1. we can have, wave like behavior of light

## Heisenberg Uncertainty principle (HUP)

The uncertainty pairs of physical properties such as position and speed cannot be simultaneously measured.

$$\Delta x \cdot \Delta p_x = \frac{h}{2\pi}$$

$$\Delta x \cdot \Delta p_x \geq \frac{h}{2}$$

$$\Delta E \cdot \Delta t \geq \frac{h}{2}$$

A student is examining a bacterium under a microscope. The *E. coli* bacteria cell has a mass of  $0.1 \text{ fectogram (}0.1 \text{ Fg}\text{)}$  and is swimming at a velocity of  $10 \text{ } \mu\text{m/s}$ , with an uncertainty of  $10\%$  of velocity of  $10\%$ .

Hint :- *E. coli* bacteria cell are around  $1 \mu\text{m}$  in length. What is the uncertainty of position of the bacteria?

solt

$$\text{mass} = 0.1 \text{ Fg} = 0.1 \times 10^{-15} \text{ kg}$$

$$\text{Velocity} = 10 \mu\text{m/s} = 10 \times 10^{-6} \text{ m/s}$$

$$\text{Uncertainty in vel} = 10\% = 0.1 \text{ m/s}$$

$$\Delta x \cdot \Delta p_x \geq \frac{h}{4\pi}$$

$$\Delta p_x = mv = (0.1 \times 10^{18}) (10 \times 10^{-6} \times 0.1)$$

$$\Delta x \geq \frac{h}{4\pi \Delta p_x} = \frac{6.626 \times 10^{-34}}{4\pi (0.1 \times 10^{18}) \times (10 \times 10^{-6})}$$

$$\Delta x \geq 0.53 \times 10^{-9} \text{ m}$$

### Basic fundamental of Q.M

i) wave function ( $\Psi$ )

- ii) Probability
- iii) Operators
- iv) Expectation value

v) Uncertainty value

vi) mathematical formalize

### Wavefunction ( $\Psi$ )

In Q.M, the instantaneous state of a system is represented by a complex wave function  $\Psi(x, t)$ . A wave function contains information about where a particle is located and it must be well behaved. i.e. It must satisfy the following:

- 1 A wave function is in general complex e.g.  $\Psi(x, t) = a + ib$
- 2 A wavefunction  $|\Psi(x, t)|^2$  is always real and not negative. In other words, it is always  $\geq 0$

$$|\Psi(x, t)|^2 = (a + ib)^2 \geq 0$$

3. A wavefunction must be single valued i.e. for each points on a domain, the wave function must be a unique value.
4. A wavefunction must be continuous i.e. the small change in the input will translate to a small change in the output. The function has finite value at any point in a given space.
5. A wavefunction must be differentiable i.e. the derivative exists and it is a continuous function.
6. A wavefunction must be square integrable - for normalization condition to be satisfied, the given wave function must be square integrable.

$$\text{i.e. } \left[ \int_{-\infty}^{\infty} \psi \psi^* dx = 1 \right]$$

If the wavefunction has a value at point  $x$ , the probability of finding the particle between  $x$  and  $x+dx$  is proportional to  $dx$ .

$$Pr \propto dx \quad \frac{|\psi|^2}{x \ dx}$$

### Probability and Normalization

#### In Quantum mechanics

The wave function that describes a quantum state provides the most complete description about the state.

$$\text{Wave function} = \psi$$

Wavefunction cannot be measured, and therefore it is seen not to have physical meaning. However, the information that can be derive from the wave function is related to the probabilities of the possible outcome of the measurement that are made on the quantum system.

$$\hat{H}\psi = \sum E_i \psi_i$$

$\psi_n \rightarrow$  Eigen values

$E_1, E_2, E_3$  are Eigen energy

The eigen functions are said to be orthonormal

- \* The Eigen function is normalized so that the probability of finding electron ( $e^-$ ) anywhere in space will be unity.
- \* Two eigen energy vectors with different eigen values are said to be orthogonal.

$$\int_{-\infty}^{\infty} \psi_i^*(x) \psi_j(x) dx = \delta_{ij}$$

$i=j \Rightarrow$  orthonormal,  $\delta_{ij}=1$

$$\delta_{ij} = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases} \quad \psi = A \sin\left(\frac{n\pi x}{L}\right)$$

$$P_r = \int_{x_1}^{x_2} \psi_n^*(x) \psi_n(x) dx = 1 \quad \text{normalization constant}$$

## Quantum mechanics Operator.

In Quantum Mechanics, application of operators are so vital because waves are being used to described dynamical systems.

"A Quantum Mechanics operator is defined as a mathematical instruction that can be performed on a wave function in order to extract a useful information about a wave function". These operators are associated with measurable quantities i.e. Observables. For instance, the energy of a particle in a quantum system can be measured. Hence energy is observed.

Other common Observables in QM are position, momentum and angular momentum. Each quantum mechanics operators

1) associated with observable

$\psi_n$ ; eigen value  $a_n$ , observable  $A$ , operator  $\hat{A}$

$$\hat{A} \psi_n = a_n \psi_n$$

→ eigen value

SN	Operators	Observable	Description or remark
1.	$\hat{A} = \hat{A}$	Unknown (generic) Observable A	This operator is for an unknown Observable A
2	$\hat{x} = \hat{x}$	Position	This operator is for position, $x$ in 1-D and $\mathbf{r}$ in 3D
3	$\hat{P}_x = i\hbar \frac{\partial}{\partial x}$	Momentum	The operator is for momentum in $x$ direction. <del>and</del> for $y$ and $z$ direction.

4. Operator	Observation	Remarks
$\hat{T} = \frac{-\hbar^2 \partial^2}{2m \partial x^2}$	Kinetic energy	For K.E of a quantum system
$\hat{V}(x) = \hat{V}(x)$	Potential energy	For P.E of a quantum system
$\hat{H} = i\hbar \frac{\partial}{\partial t}$	Time dependent Hamilton	In addition of its <del>time</del> in determining the quantum system, energies, the hamilton can also operate on a wave function to generate the time evolution of wave function.
$\hat{H} = -\frac{\hbar^2 \partial^2}{2m \partial x^2} + V(x)$	Time independent Hamilton	The time independent Schrodinger equation can be constructed when time independent hamilton operates on wave function.
$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$	Angular momentum	Angular momentum in z direction.

NB Schrodinger Wave equation

$$\hat{H}\Psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + \hat{V}\Psi(x)$$

## EXPECTATION VALUES AND UNCERTAINTY VALUES

- 1 Expectation value :- The estimate of the mean.
- 2 The uncertainty value :- The spread of the value around the mean i.e. standard deviation. Suppose that an observable quantity A, has small discrete values;  $a_1, a_2, a_3, \dots, a_n$ , then we can prepare 'n' identical system i.e ensemble of systems, all in the same state and measure the value of 'a' in each system.

In general, we will get a spread of results. In this regard the best estimate of quantity A is to get its mean value and standard deviation can be used as a measure of spread of uncertainty in the measurement.

S/N	Operator	Observable	Expectation value Integral
1.	$\hat{A}$		$\langle A \rangle = \int_{-\infty}^{\infty} \psi_n^*(x) \hat{A} \psi_n(x) dx$
2.	$\hat{x}$		$\langle x \rangle = \int_{-\infty}^{\infty} \psi_n^*(x) \hat{x} \psi_n(x) dx$
3.	$\hat{P}$	Momentum	$\langle P \rangle = \int_{-\infty}^{\infty} \psi_n^*(x) \hat{P} \psi_n(x) dx$
4	$\hat{T}$	K.E	$\langle T \rangle = \int_{-\infty}^{\infty} \psi_n^*(x) \frac{1}{2} \hat{P}^2 \psi_n(x) dx$

5  $\hat{V}$

$$\langle V \rangle = \int_{-\infty}^{\infty} \Psi_{(n)}^*(x) \hat{V} \Psi_n(x) dx$$

L  $\hat{H} = \hat{T} + \hat{V}$  Hamilton  $\langle H \rangle = \int_{-\infty}^{\infty} \Psi_n^*(x) \left( \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \hat{V}(x) \right) \Psi_n(x) dx$

$$\Psi_n^*(x) \Rightarrow \text{Bra} \quad A\Psi_n(x) = k_{ret}$$

$$\text{Uncertainty } \Delta A = [E \langle A^2 \rangle - \langle A \rangle^2]^{1/2}.$$

The wave function  $\Psi_n(x)$  cannot describe a particle that has a sharp momentum and is localized in space. The uncertainty in the measurement:  $\Delta x \Delta p \geq \frac{\hbar}{2}$

$$\Delta x = [\langle x^2 \rangle - \langle x \rangle^2]^{1/2}$$

$$\Delta p = [\langle p^2 \rangle - \langle p \rangle^2]^{1/2}$$

$$\therefore [\langle x^2 \rangle - \langle x \rangle^2]^{1/2} [\langle p^2 \rangle - \langle p \rangle^2]^{1/2} \geq \frac{\hbar}{2}$$

Assignment

1 A particle of mass  $m$  is in the state  $\Psi_n(m, t) = A e^{-\alpha t}$

$\Psi_n(m, t) = A e^{-\alpha} \left[ \frac{m x^2}{\hbar} + i t \right]$ , where  $A'$  and  $\alpha'$  are real constants  
determine the normalisation constant  $A$

Calculate the expression value of momentum and position,  
hence justify the validation and non-validation of HUP

## Mathematical fundamental of Quantum Mechanics

The basic mathematical background necessary to robust the understanding of quantum mechanics is linear algebra in infinite space i.e. Hilbert Space. With the concept of linear algebra, the state function which is in complex domain and other mathematical operation upon it are represented in simple and compact mathematical notation. In complex field theory, complex number  $z$  is denoted by  $a + ib$ , where  $a$  and  $b$  are real numbers and  $i = \sqrt{-1}$ . Here

Given complex conjugate  $z^*$  of  $z$  is  $a - ib$ . This implies that the product  $zz^*$  is a real number.

For a set of vectors  $\{x_n\}$  belongs to  $V$  [CN],  $V$  can be written as the linear combination of  $V$ 's  
 $v = a_1x_1 + a_2x_2 + \dots + a_nx_n$  where  $a_1, a_2$  are complex no while  $x_n$  are vectors and they are linearly independent, if  $a_1x_1 + a_2x_2 + \dots + a_nx_n = 0$

The vector  $x_1 + x_2 + \dots + x_n$  are called the basis and must be unique and must have the dimension of  $V$ .

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→ The complex conjugate  $z^*$  of  $z$  is  $a - ib$ . This implies that the product  $zz^*$  is a real number.

for a set of vectors  $\{x_n\}$  belongs to  $V$  [ $\in V$ ],  $v$

can be written as the linear combination of  $V$  i.e  
 $v = a_1 x_1 + a_2 x_2 + \dots + a_n x_n$  where  $a_1, a_2$  are complex no.  
while  $x_n$  are vectors and they are linearly independent, if  
 $a_1 x_1 + a_2 x_2 + \dots + a_n x_n = 0$

The vector  $x_1 + x_2 + \dots + x_n$  are called the basis and it is unique and must have the dimension of  $V$

## Dirac Function (Notation)

In Quantum mechanics, Bra and Ket notation also known as Dirac notation is a standard notation for describing quantum mechanical state. The notation can also be used to denote vectors in linear algebra. In such terms, the scalar product or action of a linear function on a vector in a complex vector space ( $\mathbb{C}^n$ ) can be represented as  $\langle b | a \rangle$

In linear algebra, the abstract vector  $C(a) \rightarrow$  to be  $|a'\rangle$  where  $|a'\rangle$  is a new vector. Similarly,  $|a\rangle + |b\rangle = |c\rangle$ . Complex numbers are themselves vector space i.e. they are column vector

$$|a\rangle = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_n \end{pmatrix}$$

$$|b\rangle = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{pmatrix}$$

$$|ca\rangle = \begin{pmatrix} ca_1 \\ ca_2 \\ ca_3 \\ \vdots \\ ca_n \end{pmatrix}$$

$$|a\rangle + |b\rangle = \begin{pmatrix} a_1 + b_1 \\ a_2 + b_2 \\ \vdots \\ a_n + b_n \end{pmatrix}$$

Every complex vector, represented as the 'ket' vector has a complex conjugate vector in a dual vector space to the original vector space (known as bra - a row-vector)

$$|a\rangle = \text{column wise} \rightarrow \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_n \end{pmatrix}$$

$$\langle a | = \text{row wise} \rightarrow (a_1^*, a_2^*, a_3^*, \dots, a_n^*)$$

The state of a QM is defined as a vector | which

belong to a hilbert space and obey the superposition principle.

is  $|\psi\rangle, |\psi_1\rangle, \dots, |\psi_n\rangle$  are ket belonging to ~~the~~ Hilbert spaces. The linear combination shown below is also a valid state vector belonging to Hilbert space.

$$|\psi\rangle = a_1|\psi_1\rangle + a_2|\psi_2\rangle + \dots + a_n|\psi_n\rangle$$

So the state function conventional rep. by a ket is a column vector that must be multiplied by a row vector known as bra.

S/N	Operator	Dirac notation for expectation value	Integral notation for expectation value
1	General $\hat{Q}$	$\langle \psi   \hat{Q}   \psi \rangle$	$\langle Q \rangle = \int_{-\infty}^{\infty} \psi_n^*(x) \hat{Q} \psi_n(x) dx$
2	Position $\hat{x}$	$\langle \psi   \hat{x}   \psi \rangle$	$\langle x \rangle = \int_{-\infty}^{\infty} \psi_n^*(x) \hat{x} \psi_n(x) dx$
3.	Momentum $\hat{P}_x$		

INNER PRODUCT, ORTHOGONALITY AND ORTHONORMALITY.

The inner product of the two vector is defined as

$$\langle b | a \rangle = (b^*, b_2^* \dots b_n^*) \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

$$= b_1^* a_1 + b_2^* a_2 + \dots + b_n^* a_n.$$

If the vectors are perpendicular to each other in orthogonality form. The inner product can be expressed as

$$\langle \alpha | \beta \rangle = \int_{-\infty}^{\infty} \phi^*(x) \psi(x) dx = 0$$

However generally the orthonormality condition is the general condition orthnormality.  $\langle \phi_n | \phi_m \rangle = \delta_{nm}$

$$\langle \phi_n | \phi_m \rangle = 1 \quad \text{if } n=l, m=l$$

$$\langle \phi_n | \phi_m \rangle = 0 \quad \text{if } n \neq m.$$

Normalization Condition

$$\int_{-\infty}^{\infty} \phi^*(x) \phi(x) dx = 1$$

For an arbitrary Quantum mechanics state  $| \psi_n \rangle$ , representing orthonormal basis vector in a hilbert Space, we can express a given state vector as a linear combination of this basis.

$$| \psi \rangle = \sum_{n=0}^{\infty} c_n | \phi_n \rangle$$

Since the basis state are orthonormal, we can defined

$|\psi\rangle$  to be equal to  $\sum_n a_n |\phi_n\rangle$

$$= \sum_n |\phi_n\rangle \langle \phi_n| \psi \rangle$$

$$= \sum_n (|\phi_n\rangle \langle \phi_n|) |\psi\rangle$$

$$= \sum_n |\phi_n\rangle \langle \phi_n| = 1$$

The equation above is the completeness equation

$|\phi_n\rangle \langle \phi_n|$  is the outproduct which defines Projection P.

Classwork.

1. The set  $\{ |1\rangle, |2\rangle, |3\rangle \}$  is an orthonormal basis in a three dimensional vector space. Let  $|\psi\rangle$  be a vector in the vector space with:  $|\psi\rangle = a (|1\rangle + 2i|2\rangle + (1+i)|3\rangle)$  and operator  $\hat{Q}$  act on vectors in a 3-D vector space with the following effect on the orthonormal basis set  $\{ |1\rangle, |2\rangle, |3\rangle \}$

$$\hat{Q} |1\rangle = |1\rangle + |2\rangle$$

$$\hat{Q} |2\rangle = -|1\rangle + |2\rangle$$

$$\hat{Q} |3\rangle = 0$$

If  $|\psi\rangle$  is a normalizable state function, find the value of constant a

$$|1\rangle \times |1\rangle = 1$$

$$|1\rangle \times |2\rangle = 0$$

i. what is the representation of the column vector for  $|1\rangle$  and  $Q|1\rangle$  in this basis

ii. write down the matrix representation of  $\hat{Q}$  in this basis?

Sohm

$$a[|1\rangle + 2i|2\rangle + (1+i)|3\rangle] \times a(|1\rangle - 2i|2\rangle + (1-i)|3\rangle) = 1$$

$$a^2 \cdot 7 = 1$$

$$a = \sqrt{\frac{1}{7}} = \frac{1}{\sqrt{7}}$$

~~$$a^2[|1\rangle + (1-i) + 2i + \dots + 2 + 2]$$~~

$$|1\rangle = \frac{1}{\sqrt{7}} (|1\rangle + 2i|2\rangle + (1+i)|3\rangle)$$

$$|1\rangle = \cancel{\begin{pmatrix} |1\rangle \\ |2\rangle \\ |3\rangle \end{pmatrix}} \quad \frac{1}{\sqrt{7}} \begin{pmatrix} |1\rangle \\ 2i|2\rangle \\ (1+i)|3\rangle \end{pmatrix}$$

Correction

$$(i) |1\rangle = \begin{pmatrix} \langle 1|\psi \rangle \\ \langle 2|\psi \rangle \\ \langle 3|\psi \rangle \end{pmatrix} = \frac{1}{\sqrt{7}} \begin{pmatrix} i \\ 2i \\ 1+i \end{pmatrix}$$

$$b) Q|\psi\rangle = \begin{bmatrix} \langle 1 | \hat{Q} | \psi \rangle \\ \langle 2 | \hat{Q} | \psi \rangle \\ \langle 3 | \hat{Q} | \psi \rangle \end{bmatrix} = \frac{1}{\sqrt{7}} \begin{pmatrix} 1-2i \\ 1+2i \\ 0 \end{pmatrix}$$

III.  $\hat{Q} = \begin{bmatrix} \langle 1 | \hat{q}_1 | 1 \rangle & \langle 1 | \hat{q}_1 | 2 \rangle & \langle 1 | \hat{q}_1 | 3 \rangle \\ \langle 2 | \hat{q}_1 | 1 \rangle & \langle 2 | \hat{q}_1 | 2 \rangle & \langle 2 | \hat{q}_1 | 3 \rangle \\ \langle 3 | \hat{q}_1 | 1 \rangle & \langle 3 | \hat{q}_1 | 2 \rangle & \langle 3 | \hat{q}_1 | 3 \rangle \end{bmatrix}$

$$= \begin{bmatrix} 0 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$