# PH 203: Quantum Mechanics - I

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R. Feynmann Lecture notes.

Grading: 6 chapters + 1 introductory chapter.
⇒ 6+1 Homeworks.

- H.W: - 30 %
- Midterm: 30 %
- End term: 40 %

History: • For a long time, much before the modern science, people had evidence and wondered about what are the most fundamental quantities, and why they come in quanta/discrete values. And what quantities can take discrete values? Like energy, momenta, charge, but not mass etc.

• Greek thinker in 500 BC proposed that matter is composed of atoms and the name itself came from the Greek time. In the Egyptian time to Greek time, people, especially the Alchemists, measure volume of different elements and they come in some multiples of discrete number. Boyle propose empirical relation of $PV = nRT$, where $R = N_A k_B$, for n mole ideal gas in which $N_A$ number of molecules per mole exists. So, all ideal gas made of fundamental discrete particles. Kelvin proposed atoms are topological vortices in the ether medium in 1865. With the advent of experimental probes, people were able to visualize what's inside an atom.

After the discovery of radioactive element, Rutherford in 1911 showed that atoms are mostly empty with most of its mass concentrated at the center. It was Bohr who eventually had the proposal of electrons circulating the nucleus of positive charges. The charge and spins were discovered by Thompson and Stern-Gerlach experiments, both take discrete values. Finally, the wave properties of the electrons was proposed and measured by double-slit experiment.

- Experiments with light also started long before. But earlier the apparatus did not have the slit size small enough to the order of magnitude of the light's wavelength to probe single wave, and hence its particle like nature. Newton in fact had a proposal that light is made of particles. Perhaps he did not have the same concept in mind that what we call photon today. But during that time, other experiments showed interference / diffraction patterns which suggested the wave nature of light. The history of ether medium required for the wave to propagate is known to everybody. In fact Lord Kelvin thought the knot structure in the ether medium produced atom. Thanks to Maxwell's equations, in which he reconciled the electric and magnetic fields, he showed that there can be electromagnetic wave in free space. This was the key theory which helped abandon the ether proposal. By 1859, Kirchhoff and others found a relation between wavelength & temperature which cannot be explained by classical / statistical theory - called black body radiation. Then photoelectric effect showed discrete energy of light. Compton effect and Raman effects were key for particle nature of light as these experiments could be understood by scattering of particles theory in which momentum is transferred.

(i) By 1859 and later, Kirchhoff and others made series of experiments with light and found unusual dependence of intensity, wavelength and temperature - the black body radiations. This result could not be explained by classical theory of continuous energy spectrum of light. Planck had a proposal that energy is proportional to frequency as $E = h\nu$, where 'h' is called the Planck's constant. Later on, Einstein also used this hypothesis to explain the photoelectric effect. Therefore, these two experiments suggest energy comes in discrete amount, like packet of energy. These two experiments are not yet enough to assign each packet of energy to a particle. Particle description would require momentum (not necessarily mass though as we know from Einstein theory of relativity).

(ii) Next came Compton & Raman effects, where one observe scattering like behavior of light / lattice vibrations, which has momentum transfer. Now, momentum transfer is not something that we usually say for a wave, rather for scattering between particles. A notion of energy packet of waves behaving like particle starts to emerge. What is the momentum of this particle then? De Broglie had a similar hypothesis, although later but its more appropriate to introduce here, that the momentum of the particle is proportional to the inverse wavelength of the wave, and the proportionality constant is again 'h', i.e., $p = h/\lambda$. Therefore,

the momentum is also discrete and comes in packet. Because, frequency & wavelength are related to each other for plane waves as $c = \lambda\nu$, so a relation between $E$ & $p$ is obtained as $E = pc$. This is not consistent with Newton's equation where $E = p^2/2m$, but this is consisted with relativity for massless particles. So the packet of energy and momentum of light and vibrations are called photon & phonon, which are particles.

(iii) So far so good. But how about the interference and diffraction pattern? Mach-Zender interferometer experiment (1891-92) was done with a beam of light split into two beams, and then again the two beams are combined which then show interference pattern with intensity being maximum and zero at different locations. If we try to explain this in terms of photon, there is a problem. Lets say, the beam is made of many many photons, and in the beam, half of the photon goes in one path and another half in the other path. But upon recombination of the two beams, how come there is a destruction of the intensity, which would mean the photons are annihilated, and its energy vanished? Similarly, at the maxima of the intensity, new photons are created? This does not actually makes sense. (There were some other proposals by Einstein and others saying photons have some

hidden variable and degrees of freedom etc, but those theories did not holed longer). The correct theory begin to emerge is that interference (or rather diffraction) is rather made by a single photon alone, which is defined not completely defined to be localized at a given position at a given time like a classical particle, but its like a "vector" (to be called state vector or wavefunction or simply a function of space-time to begin our discussion). Therefore, as a "vector" can be defined by two linearly independent unit vectors in 2D with the components denoting how much the amplitude of the vector is present along each unit vector. Similarly, we have learned from the vector space that a function can be expanded in terms of linearly independent set of functions, called vector space. In the above interference phenomena, the photon's dynamics should still be described by a "wavefunction" and when it splits by the beam splitter into two, it means we are now expanding the "wavefunction" into two linearly independent "wavefunctions", $\psi(x) = c_1 \phi_1(x) + c_2 \phi_2(x)$, with the coefficient of expansion $c_1, c_2$ measuring the probability of the photon being in the corresponding states. This means, the same photon has finite probability of being in two beams (states) here. $\phi_1$ & $\phi_2$ interfere.

This gives rise to the superposition principles, and hence a probabilistic approach is necessary and we have to abandon the deterministic approach of classical mechanics.

Some people like Einstein agreed with the first two proposals $E = h\nu$, $p = h/\lambda$, but did not agree with the superposition / probabilistic approach. Later on, with electrons a similar Mach-Zehnder experiment was performed which is called double-slit experiment, and a similar interference / diffraction pattern was observed. In fact, much later, people have been able to do the interference pattern with single photon / single electron at a time which still shows the same interference / diffraction pattern, but with much lower intensity. Therefore, it is understood that the intensity in the interference / diffraction pattern counts the number of photon, not the energy itself as wave theory propose. This proves the superposition / probability (or entanglement theory in modern language) to be correct.

(*) (i+ii) Similar journey was there inside the atoms where simple classical mechanics could not explain the stability of oppositely charge particles in an atom, defying Coulomb attraction. Also the discrete values of energy absorption & emission point towards discrete nature of energy eigenvalues. Bohr postulated that the angular momentum of electron in an orbit is proportional to some integer and the proportionality constant is 'ħ', $L = n\hbar/2\pi$, where $n$ = integer. Therefore, the energy is also quantized. Later on, Stern-Gerlach experiment also came by, showing the spin angular momentum of electron is quantized in half integer unit of ħ as $S = \hbar(1/2)/2\pi$. So, quantization of energy, angular momentum of independent particles (not photon) is hence established.

(iii) Double slit experiments with electron beam shows interference pattern, establishing the superposition/probabilistic interpretation of photon to hold for electrons. So, a wave nature of particle is hence conjectured in the reverse way of particle nature of light was conjectured.

( (i) & (ii) in both cases about energy, momentum & angular momentum quantization hypothesis constitute the Old QM. (iii) in which superposition principle is used to develop wavefunction and its EOM constitute the Modern QM.)

As charge of the electron, and later on proton etc were discovered, it got many people, like Dirac wondered, why charge of a particle takes discrete values and also why the particle holds its value of charge. In other words, why the charge of a particle is conserved? The same question people ask about electron's spin, after its discovery in Stern-Gerlach experiment that, why electron's spin takes discrete values? Discrete values of some quantities and they are being conserved (means time-independent) are very much the same question. Because, during the creation of these particles, they assume some values of charge, spin, etc and they hold on to those values forever. And, when these particles move, it takes discrete values of momenta & energy. For example, when a charge particle moves, it creates electric & magnetic fields, and then when another charge particles come nearby, they interact, the fields gets screened or modified. But the charge of the particle remains the same. This is as if the particles adjust the electric & magnetic fields to keep the charge fixed. The same for spin. Similarly, in classical trajectory of motion, the particle takes those trajectories which are stationary (least action principle). As we will see, when we draw the trajectory in a phase space in the Hamiltonian formalism, the trajectories in the space will be quantized to take discrete energy, momenta etc. So does orbital angular momentum in an orbit becomes quantized. On the other hand, there are many quantities, such as mass of the particle, electric, magnetic fields do not take discrete values and are also not conserved.

(iv) Uncertainty principles

So, why some quantities are quantized, but others are not? What determines which quantity will be quantized and conserved? There is a symmetry principle behind it. Recall the Noether's theorem from classical mechanics. Space and time translational symmetries of a Lagrangian demand momentum and energy, respectively, are conserved. Noether theorem does not give momentum or energy to be quantized though. That quantum theory does. Similarly, angular momentum, spin, charge being conserved require some symmetry. Angular momentum correspond to rotational symmetry in an orbit. Spin and charge quantization are purely quantum mechanical phenomena, requiring the description of a complex wavefunction, which as rotational and phase (gauge) symmetry. We can intuitively think of it as as the theory is invariant with any value of position, time, rotation, phase etc, then the trajectory of a particle make use of this liberty to adjust the space, time, angle, phase to keep their corresponding quantity

conserved. Notice that the corresponding quantity is the canonical momentum or canonical variable, such as space translation correspond to momentum conservation etc. The two variables which are canonically conjugate to each other gives the Hamiltonian description which gives the trajectory in the phase space. We will see that behind all the discrete / quanta nature of these quantities, there is a general principle that the phase space is not continuous, but consist of discrete grid of of area 'h', where 'h' is called the Planck's constant and has the dimension of '$px$', '$Et$', '$L\theta$', i.e. the phase space area. There is no fundamental principle or mechanics that we can find out why the phase space is discretized and why we can not shrink the phase space to zero, i.e., why $h$ cannot go to zero. But if we make this hypothesis or assumption, we can obtain all results that are consistent with experiments. Needless to say, we can appreciate the discrete nature of the phase space in the values of position & momentum are such that $px \sim h$, then we will see the quantum behavior ($h \sim 10^{-23}$). At large length scale, we won't have to resort to see the discrete nature of the phase space, and the trajectory will look continuous (classical).

- What the above discretization of the phase space is also suggesting is that, within a specific grid, the theory is very much invariant or the position & momentum are not completely known at least upto a lowest possible phase space grid size of $\Delta x \sim h$. This leads to uncertainty in position-momentum and between any variable and its canonical conjugate variable whose product is restricted by the minimum possible phase space area $h$.

- We see that while in classical mechanics, we evaluate the coordinates of particles in time $x(t)$ via some equation of motion, in quantum Theory we will introduce a complex function $\psi$ which is defined in space time, i.e $\psi(x,t)$. There will be an equation of motion to describe the evolution of the wave function, called Schrödinger equation. By this new formalism of describing an equation of motion via an abstract function brings in new symmetry associated with the wave function $\psi(x,t)$ such as phase (gauge) symmetry which was not present in the classical Noether theorem. Examples of these extra symmetries are phase (gauge) symmetry giving charge conservation, exchange symmetry due to identical particles etc. We will not be able to cover this entire framework in QM-1, but by the end of QM-3 & QFT course, you will have a full understanding of all these concepts.

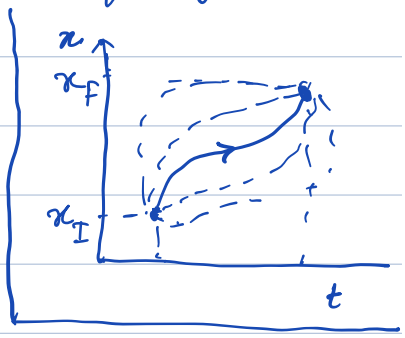
- And because of the underlying uncertainty is the phase space and since the theory will be defined by an abstract complex function, $\psi(x,t)$ which is not not even measurable, we need to abandon the deterministic approach, and resort to a probabilistic approach. We will define a probability density $\delta(x)$ in terms of the complex function $\psi(x,t)$. We finally need a prescription to compute physical / measurable quantities from this probability density, such as average / expectation value. An analogous but not the same probabilistic approach was taken in the statistical mechanics.

- Finally we need to make sure the new theory we build must reproduce all the other fundamental conservation laws, such as continuity equation of charge density (~ probability density) and current density (probability current) that we obtain, for example, from the Maxwells equations. Finally all the quantum theory must reproduce the classical theory in the mathematical limit of $\hbar \to 0$, as Bohr hypothesized. This rule is called Bohr's correspondance principle. We will also see in occasions that the average (expectation values of physical / measurable quantities in some cases follow classical equations - Ehrenfest theorem.

# Recap : Classical Mechanics.

⊛ **Newtonian Mechanics**: This gives us an equation of motion to solve for a particles's trajectory $x(t)$, given we know its past immediately before in time $t_0 < t$. Because here we solve a second order PDE which solves for $x(t+\varepsilon)$ given we know $x(t-\varepsilon) \& x(t)$ where $\varepsilon$ is infinetesimally small. We solve the eq. of motion for each individual particles $x_i(t)$ by knowing all the forces acting on it.

⊛ **Least Action Principles**: In the least action principle or the stationary state solutions, we know the initial and final positions $x^I(t) \& x^F(t)$ and we define all possible trajectories defined by a Lagrangian $\mathcal{L}(x, \dot{x})$ and solve for the stationary state trajectory which minimizes the action $S = \int dt\, \mathcal{L}$. The stationary state solution gives us the equation of motion that Newton predicted.




⊛ **Noether's Theorem**: Noether theorem tells us that for every continuous symmetry, there is a conserved quantity. Continuous symmetry means under a continuous transformation, the action remains invariant. For example, under time translational symmetry, the total energy (ie, Hamiltonian) is conserved. For space translational symmetry, the

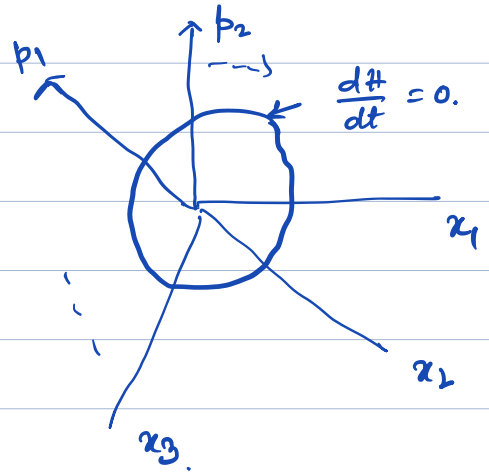
momentum is conserved. Under rotational symmetry, angular momentum is conserved. Importantly, these conserved quantities are only conserved on the stationary path. So, the particle moves on the path which conserve energy, momentum or angular momenta if the corresponding symmetry is present. This actually plays an important role in all branches of physics.

(*) Hamiltonian principles: The Hamiltonian (= total energy) is a function of $x_i$ & $p_i$, ie, it's defined in the phase space $(x, p)$. Here we study the dynamics of the particle in the phase space on a constant energy path:

$$\frac{d}{dt} S(p,q) = \frac{d}{dt}(p\dot{x} - H) = 0.$$

which gives the Hamiltonian equation of motion (one may call it)

$$\dot{x}_i = \frac{\partial H}{\partial p_i} \quad ; \quad \dot{p}_i = -\frac{\partial H}{\partial x_i}$$



## Poisson Bracket:

Def: $\{A, B\}_{P.B.} = \sum_i \left( \frac{\partial A}{\partial x_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial x_i} \right)$

- $\frac{dA}{dt} = \{H, A\} + \frac{\partial A}{\partial t}$.

  When $A$ doesn't have any explicit time-dependence, i.e., $\frac{dA}{dt} = 0$, we have $\frac{\partial A}{\partial t} = \dot{A} = \{A, H\}$.

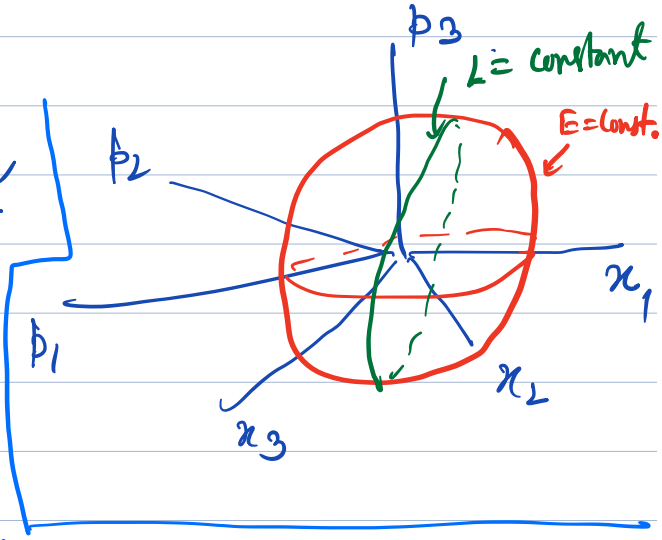
- This gives

  $\dot{x}_i = \{x_i, H\} = \frac{\partial A}{\partial p_i}$ ; $\dot{p}_i = \{p_i, H\} = -\frac{\partial H}{\partial x_i}$

- $\{x_i, p_j\} = \delta_{ij}$

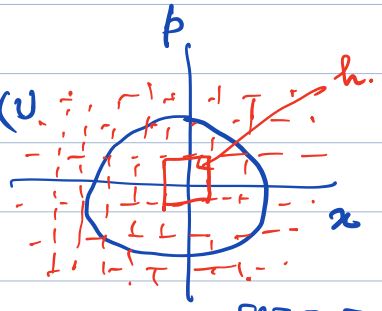
  This non vanishing Poission bracket between $x$, $p$ implies that $x$ & $p$ are no longer independent variables, but becomes related to each other as the particle follows the equation of motion / least action principle.

- A conserved quantity, say energy, constraint the trajectory in the phase space on a constant energy surface (like the red hypersphere). If we have another conserved quantity, say linear or angular momentum, then the motion is further restricted to the crossection of the two constant surface. If $A$ is conserved, i.e. $\frac{\partial A}{\partial t} = 0 \Rightarrow \{A, H\} = 0$. If $B$ is also conserved, i.e. $\{B, H\} = 0$. Then $\{A, B\} = 0$ (show).



⊛ Bohr-Sommerfeld introduced a quantization condition for a closed (periodic) motion of particles in the phase space

$$\oint p\, dx = n h \quad \text{---(1)}$$




where $h$ is a constant, called Plack's constant, having the dimension of $[p][x] = [E][t] = [L][\theta]$ etc., the dimension of the phase space volume = [Action]. Although the above quantized orbit condition was introduced in an ad-hoc way, we can try to make sense of it as follows. The action is

$$S = \int dt \left[ p\dot{x} - H \right].$$

Assume the particle has a periodic motion with a time period of $T$. Since the particle traverse in the least action, so we have $\delta S = 0$. This implies

$$\oint p\, \dot{x}\, dt = \oint p\, dx$$
$$= \int_0^T dt\, H = T E.$$

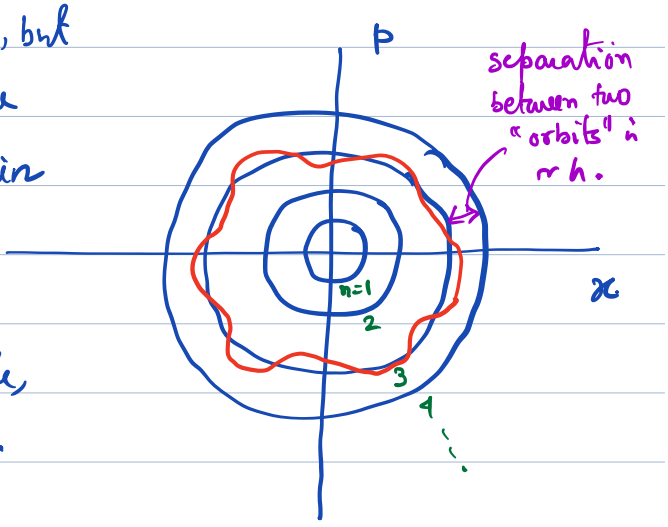
where $H = E$ is assumed a constant of motion.

The frequency $\nu = 1/T$. Then we get

$$\boxed{E = n h\nu} \quad \cdots (2)$$

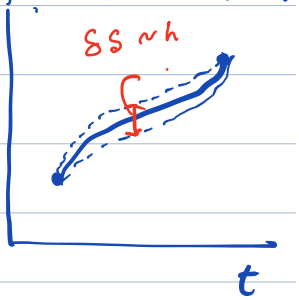
(i) This says, the Bohr-Sommerfeld condition suggests that the energy is quantized and its quantized in terms of frequency.

(ii) It also says that not all orbits in the phase space are allowed, but only those orbits whose energy is integer multiple of $h\nu$ are allowed. Considering the case of $n=1$, it is obvious that the phase space volume element ($\sim \Delta p \Delta x$) cannot be made arbitrarily small, but the minimum phase space volume grid one can obtain is $\sim h$. This is actually true for any variable and its conjugate variable, ie, $\Delta E \Delta t$, $\Delta\theta \Delta L$, etc. This actually leads to the famous Heisenberg Uncertainty principle that we will see later.




(iii) At a given energy corresponding to a value of $n$, the area under the curve is conserved and quantized and one cannot continuously go from one orbit to another

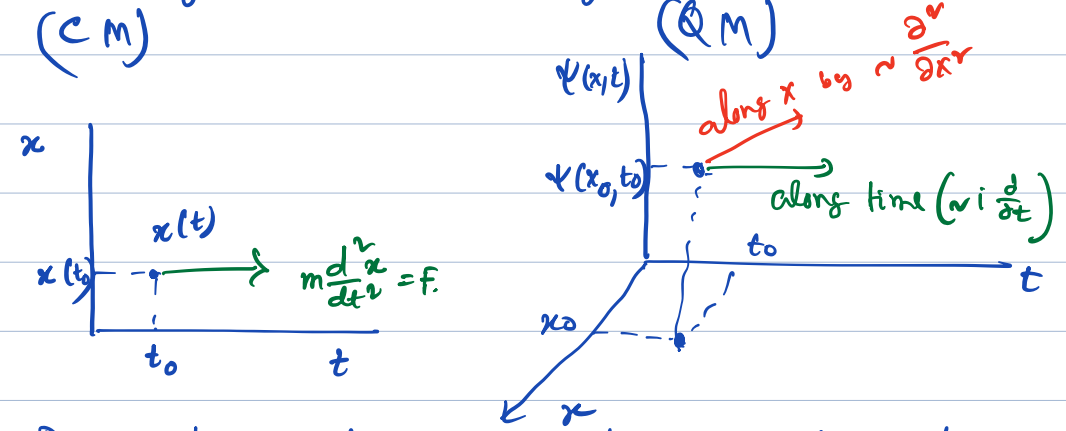
orbit. The area is conserved, but the shape of the curve is not. One can deform the closed path continuously as long as the area remains the same as illustrated by the red line on $n=3$ orbit. The maximum deformation allowed is $< 2h$ without changing the orbit and hence without violating the quantization condition. Therefore, the energy is allowed to fluctuate upto $\Delta E < 2h/T$, or the time period is allowed to fluctuate upto $T < 2h/\Delta E$. This is called quantum fluctuation which is allowed even at the stationary solution. This is another manifestation of the uncertainty principle that we will keep coming in our future discussions. This means $p, x$ can also fluctuate $\Delta x \Delta p \sim h$.




This means the least action or stationary path also can fluctuate $\sim h$ (action has the dimension of $h$). Or the minimum action $\delta S$ that we set to be zero in classical mechanics, becomes $\sim h$ in quantum mechanics. We however don't study quantum mechanics by an extention of the least action principle, but rather by an equation of motion called Schrödinger equation. The action principle of quantum theory is called path integral approach which you will learn in QM 3 or QFT.

## ⊛ A brief prelude to Modern QM (chapter 2)

- In classical Mechanics, we looked into each particles coordinates $x_i(t)$ and study how $x_i(t)$ evolves in time by solving Newton's eq involving double time-derivative.




In quantum mechanics, we change the perspective. Here we look at a general position $x$ at a time $t$, and ask what's the probability of a particle to visit that position at that time $t$. Unlike in stat physics, which is also a probabilistic approach, here we define the probability via a complex function $\psi(x,t)$ which we will call wave function. While $x(t)$ evolves by a 2nd derivative in time only, $\psi(x,t)$ will evolve by a first derivative in time, but a 2nd derivative in space (This is true for non-relativistic particles). This equation of motion for $\psi$ is called the Schrödinger eq. Anything we measure in QM is an expectation value / average under this "probability distribution".

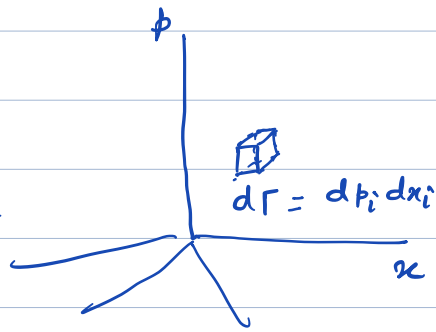
- In quantum mechanics, we replace Poisson bracket with commutator

| C.M. | | Q.M. |
|---|---|---|
| $\{A, B\}_{P.B}$ | $\longrightarrow$ | $[A, B] = AB - BA$ |
| $\{x_i, p_j\}_{P.B} = \delta_{ij}$ | $\longrightarrow$ | $[x_i, p_j] = i\hbar\,\delta_{ij}$ <br> $[\hbar = h/2\pi]$ |
| $\frac{dA}{dt} = \{H, A\}_{P.B} + \frac{\partial A}{\partial t}$ | $\longrightarrow$ | $\frac{dA}{dt} = i[H, A] + \frac{\partial A}{\partial t}$. <br> (Heisenberg's quantum Mechanics) |

(We call $A, B, H, \ldots$ operators which operates on functions and give another function).

## Recap: Statistical Mechanics & Probability.

- In statistical mechanics, we introduce a probabalistic approach. Although the approach is somewhat different, it is worth looking at it. Here also instead of looking at individual particle's $x_i$, $p_i$, which has $6N$ degrees of freedom, we look at a position & momentum and ask how many particle visits that phase space point.
We call that ensemble probability density. It denotes the # of particles $dN$ out of total number $N$ that visits the volume element $d\Gamma$ at time $t$ : $\frac{dN}{N} = \rho(x, p)\, d\Gamma$.




$\rho$ = Prob. density.

Then since $\int_\Gamma dN = N$, so we get $\int_\Gamma \rho\, d\Gamma = 1$.

Therefore the total probability inside the entire volume is 1.

- Note that the minimum phase space volume in quantum mechanics is $\hbar$, i.e., $dp\,dx \sim h$, so, $\Gamma = h^{3N}$, where $N$ = total number of particles.
- At equilibrium, $\rho_{eq}$ does not change in time. This means $\frac{\partial \rho_{eq}}{\partial t} = 0 = \{\rho_{eq}, H\}_{P.B.}$

So, $\rho_{eq}(H=E)$ is a function of energy, or have a zero Poisson bracket. If we have more conserved quantities, say angular momentum, $H$, and $\rho_{eq}$ have a vanishing Poisson bracket with all the conserved quantities.

- **Mathematical treatment of probability & averages:**

→ Let us say $\rho(x,t)$ is a probability density of having a particle visiting the interval $x$ & $x+dx$ at $t$. Then the total probability that the particle lies between the interval $[a,b]$ is

$$P_{ab}(t) = \int_a^b \rho(x,t)\,dx.$$

→ The total probability of that the particle lies in the entire space is 1:

$$\boxed{\int_{-\infty}^{\infty} \rho(x,t)\,dx = 1}$$

[Normalization condition].

(we notice that the right hand side does not have any time dependence).

Therefore, the time dependence of the probability must follow a proper equation of motion such that the total probability in the entire space is zero. In other words, we are assuming there is no source or sink to create and destroy particle in the entire space. In other words, we are assuming the total number of particle is conserved. If there was a source or sink of particle, there would be a divergence of probability current $\vec{J}$, coming out/in to the source/sink. Therefore, the above statement says, the evolution of the prob. density follow the continuity equation

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

→ The average value of a measurement $f(x)$ with this probability distribution is

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x)\, \rho(x)\, dx .$$

[e.g. $f(x) = x$, $E(x)$ = energy density, $\rho(x)$ = mass density]

→ The variance or standard deviation of the measurement is

$$\Delta f = \sqrt{\langle f^2(x) \rangle - \langle f(x) \rangle^2} .$$

→ In modern quantum mechanics, we are going to define the probability density by the amplitude of the wave function. ∞

$$\rho(x,t) = |\psi(x,t)|^2 = \psi^*(x,t)\,\psi(x,t).$$

Then $$\int |\psi(x,t)|^2 dx = 1.$$

$$\langle f(x) \rangle = \int \psi^*(x,t)\, f(x)\, \psi(x,t)\, dx$$

(The normalization condition again puts a restriction on the time-evolution on $\psi(x,t)$ such that it always normalizes to 1. Do we get a continuity equation of $\psi^2$? Yes.).

[ Since $\rho \sim \psi^*\psi$ is the physical quantity, so, the phase $\phi$ of $\psi = |\psi| e^{i\phi}$ can be arbitrary. This is called a gauge symmetry.

H.W.

Study Gaussian / Poisson distributions:

## Recap: Electricity & Magnetism.

Maxwell's equations:

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

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

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

$$\vec{\nabla}\times\vec{B} = \mu_0\vec{J} + \frac{1}{c^2}\frac{\partial\vec{E}}{\partial t}$$

### Free space (Wave equation)

$$\frac{1}{c^2}\frac{\partial^2\vec{E}}{\partial t^2} - \nabla^2\vec{E} = 0.$$

$$\frac{1}{c^2}\frac{\partial^2\vec{B}}{\partial t^2} - \nabla^2\vec{B} = 0$$

Solutions: $\vec{E}(\vec{r},t) = \vec{E}(0,0)\, e^{i(\vec{k}\cdot\vec{r} - \omega t)}$ — (1)

$$\vec{k} = \frac{2\pi}{\lambda}, \quad \omega = 2\pi\nu.$$

$\omega^2 = k^2/c^2 \Rightarrow c = \nu\lambda$.

(Plane wave solutions).

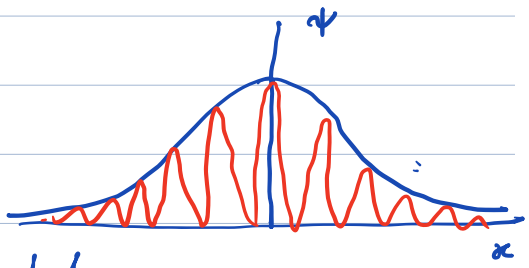
### In a medium (Continuity equation)

(If the electromagnetic fields arise from the dynamics of charge particles, we get the continuity equation:

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0.$$ — (2).

- Although here wave eqn & continuity eqns are for EM wave (light) and for charge particles, but when we quantize a wave and define particle density $\rho \sim \psi^*\psi$, it must follow the continuity equation. Schrödinger indeed started with a prediction that $\rho = \psi^*\psi$ follows eqn (2) while $\psi$ follows a equation such that its solution follows eqn (1) when there is no potential (free particle)

- But the first hurdle is clearly, the plane wave gives $\rho(x,t) = \psi^* \psi = e^{-i(\vec{k}\cdot\vec{r} - \omega t)} e^{i(\vec{k}\cdot\vec{r} - \omega t)} = 1$. So, the probability is constant everywhere. This is however a problem then. The plane wave is oscillatory everywhere and is spread over all time & space. So, we need to localize the wave within a certain range to be able to describe a particle. So we need damping to localize a wave and/or a standing wave condition (confining potential) etc.




- This will be called wave packet.

(Note that plane wave to wavepacked solution will be not be done for photons, but for other particles which experience some potential energy. Plane-wave solution means solution of only kinetic energy and no potential energy. Potential energy tend to confine the wave and create wavepacket.)

H.W: : Derive wave equation and solution.
Derive continuity equation.

## Recap: Math preliminary:

- → 2nd order PDE.
- → Linear Algebra
- → Fourier transformation (delta fn, plane wave solutions)

- A second order (linear, homogeneous) differential equation has two linearly independent solutions. Therefore, any linear combination of the two solutions is also a solution of the 2nd order PDE.

  e.g. $a(x)\frac{d^2}{dx^2}\psi + b(x)\frac{d}{dx}\psi + c(x)\psi = d\,\psi(x)$.

  has two solutions $\psi_1$ & $\psi_2$.

  Then $\psi(x) = c_1\psi_1(x) + c_2\psi_2(x)$ is also a solutions of the ODE as long as $\alpha$ & $\beta$ do not depend on $x$.

Therefore, when a classical mechanics has unique solutions, quantum mechanics can in principle have infinite number of solutions - This is called superposition principles. Of course, there are physical boundary conditions and the normalization condition $\int \psi^2 dx = 1$ which put restrictions on $\alpha$ & $\beta$.

- ## Fourier Transformation :

Fourier transformation is a special type of expansion of a continuous, differentiable function in a set of linearly independent basis functions (vector space). What is special about the Fourier transformation is that the basis functions we choose are plane-wave basis: $e^{i(\vec{k}\cdot\vec{r} - \omega t)}$.

So, $$\psi(x,t) = V\int \frac{d^3k}{(2\pi\hbar)^3}\frac{d\omega}{(2\pi\hbar)} \phi(k,\omega)\, e^{i(\vec{k}\cdot\vec{r} - \omega t)} \quad \text{--- (1)}$$

($p = \hbar k$, $E = \hbar\omega$)

where $\phi(k,\omega)$ are called Fourier components or modes of $\psi(x,t)$.

The inverse Fourier transformation is

$$\phi(k,\omega) = \int d^3r\, dt\ \psi(x,t)\, e^{-i(\vec{k}\cdot\vec{r} - \omega t)} \quad \text{--- (2).}$$

Identifying $e^{i(\vec{k}\cdot\vec{r} - \omega t)}$ as the solutions of wave equations, we can interpret eq (1) as an integration over all possible wavevector $k$ or wave length $\lambda$ and frequencies $\omega$.

(For dimensional reasons, some books multiply by $V$ = volume of space, and other books ignore. In the latter case $\phi$, $\psi$ have different dimension. Also some books distribute the factor $1/(2\pi\hbar)$ between the F.T. and the inverse F.T. as $1/\sqrt{2\pi\hbar}$ on both eqn (1) & (2). It is just a matter of convention and one needs to be consistent.)

To have the dimension of $\psi$ & $\phi$ be same, we need to divide by the dimension of the phase space $[px]$ for each space-time. We divide by a constant $\hbar = h/2\pi$, where $h$ has the phase space dimension, called Planck's constant.

- We have already seen that the frequency of a wave is related to its energy as $E = h\nu = \frac{h}{2\pi} 2\pi\nu = \hbar\omega$. (for a given $n$). So, the Fourier transformation in going from time to frequency domain is equivalent to going from time to energy variables, which are sort of conserved variables to each other as we had learned from Noether's theorem. If the system has time-translational symmetry, then energy is conserved. Let us impose a periodic boundary condition on time that $\psi(t+T) = \psi(t)$, where $T$ = Time period. Then we find from the right hand side that $e^{i\omega T} = 1$, i.e.

$$\omega T = 2\pi n.$$

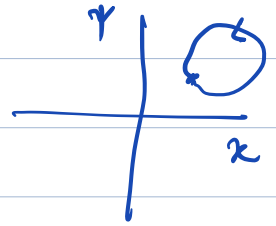
$$\text{or } \omega = \frac{2\pi n}{T} = 2\pi n\nu.$$

Then $\boxed{E = \hbar\omega = nh\nu}$. ---(3)

- Similarly (heuristically), we see that the position variable have been Fourier transformed to all possible wave vectors $k$ (inverse wavelength). So, we can identify the wavelength & wavevector by the conjugate variable to the position, i.e., the momentum $p$. This analogy gives us the de-Broglie's hypothesis that

$$p = h/\lambda = \hbar k. \quad \text{---(4)}.$$

One may also be able to derive the Bohr Sommerfeld quantization condition but not very rigorously though. Suppose there is a periodic boundary condition on the position space also. Then on the path, momentum is a function of position $\vec{p}(\vec{r})$. Then we want $\psi$ to return to its initial value after a periodic motion. This is possible when



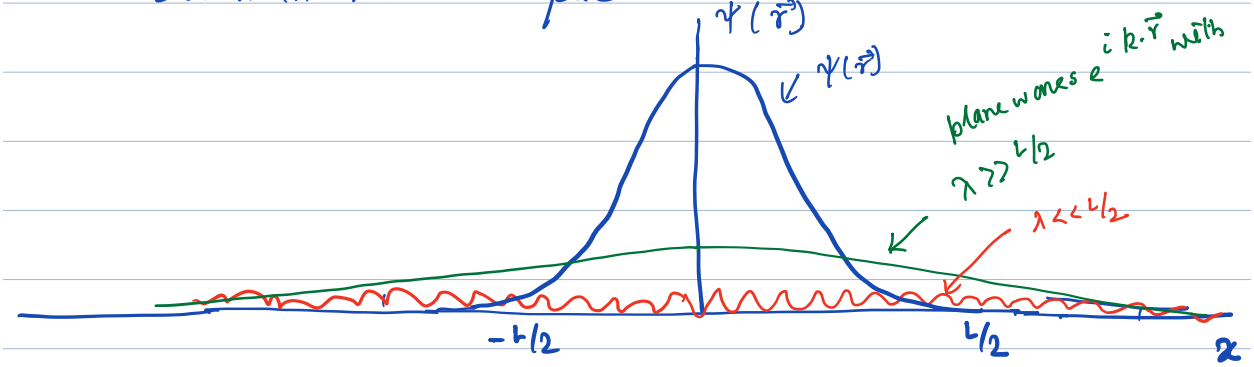

$$e^{i \oint \vec{k}(r) \cdot d\vec{r}} = e^{i \oint \frac{\vec{p}(r)}{\hbar} \cdot d\vec{r}} = 1.$$

$$\Rightarrow \frac{1}{\hbar} \oint \vec{p}(r) \cdot d\vec{r} = 2n\pi \Rightarrow \boxed{\oint \vec{p} \cdot d\vec{r} = n\hbar}$$

Notice that we did not talk about $\phi(k, w)$, therefore this above discussion is not rigorous. More careful calculation requires putting periodic boundary conditions on $\phi(\vec{k}, w)$.

- Eq (1) actually gives a hint on how to confine a plane wave solution into a finite length/volume. This can be done by choosing a functional form of $\phi(k, w)$ such that it peaks sharply at a particular

wavevector / momentum $k_0$ and decays sharply as the wavevector / momenta deviates from this value. This reduces the contributions from those plane waves which are far from $k_0$. So, $\phi(k, \omega)$ carries the weight or contributions of each plane waves with different wavelength / wavevector / momentum which are no longer equal. So, $|\phi|^2$ gives the probability distribution in the momentum space while $|\psi|^2$ gives the probability distribution in the real space.




- Suppose we want to confine the wavefunction $\psi(x)$ within the limit of $-L/2$ to $L/2$. Then from eqn (1), it's clear that those plane waves with shorter wavelength $\lambda << L$ will have lesser contributions (like the red wave) while the larger wavelengths $\lambda >> L$ will have much higher contributions. Because for confinement, you want to reduce the beating / oscillations. This is how $\phi(k, \omega)$ will be distributed among all possible wavelengths. For example, if $\psi(x)$ is completely localized at a position $x_0$, i.e, $\psi(x) = \delta(x - x_0)$ then we have

$$\delta(x-x_0) = \int \frac{dk}{(2\pi)} \; e^{ik(x-x_0)} \qquad -(3)$$

in which $\phi(k) = 1$, therefore all wavelengths contribute equally. Therefore, if the position of $\psi$ is completely known its wavelength and hence momentum is completely unknown. On the otherhand, if the function $\psi(x)$ is completely spread out over the entire space then it can be described by one plane wave $e^{ik_0x}$ & hence only $\phi(k_0) = \delta(k-k_0)$. Therefore, its momentum is completely known. Therefore, both position and momentum cannot be known completely in this wavefunction description of quantum theory. This is related to Heisenberg uncertainty principle.

(*) Can we get a bound on the uncertainty in both position and momentum (and similarly on energy & time or between any variable and its conjugate or Fourier variable)?

Recall a Gaussian probability distribution

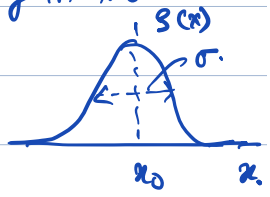
$$g(x) = \frac{1}{\sqrt{\pi\sigma}} e^{-(x-x_0)^2/\sigma} \qquad ---(4)$$

- This distribution is normalized.

$$\int_{-\infty}^{\infty} g(x)\,dx = 1$$

- The average $\langle x \rangle = \int_{-\infty}^{\infty} x\, S(x)\, dx = x_0$.

- The standard deviation / variance / uncertainty in the measured value of $x_0$ is




$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sigma. \quad -(5)$$

(*) So, lets take an example:

If we want to obtain a distribution of particle's position in space centering around $x_0 = 0$ (as an example), we choose the wave function to be (ignore the time-dependence).

$$\psi(x) = \frac{1}{(\pi\sigma)^{1/4}} e^{-x^2/2\sigma} \quad \cdots (6).$$

(we set the complex phase of this function to be uniform and set it to be zero. Because phase does not contribute to discussions below.).

- The probability distribution in real space is $S(x) = \psi^* \psi$
The fourier transformation of the "probability density" in the momentum space $P(k)$ (from eq 2) is

$$P(k) = \int dx\; S(x)\, e^{-ikx} \quad \cdots (7)$$

$$= \frac{1}{\sqrt{\pi\sigma}} \int e^{-x^2/\sigma - ikx}\, dx.$$

$$= \frac{1}{\sqrt{\pi\sigma}} \sqrt{\pi\sigma} \cdot e^{-\frac{\sigma}{4}k^2}$$

$$= e^{-\sigma/4\, k^2} \quad \text{-- (8)}$$

So, we get a Gaussian probability centering around $k=0$ and variance $\sigma_k = \frac{4}{\sigma} \cdot \frac{\pi}{4} = \pi/\sigma$ [after normalizing $P(k)$]

So, $\langle k \rangle = 0$. & $\Delta k = \sigma_k = \frac{\pi}{\sigma}$ (9)

So, from eqn (5) & (9) we get

$$\Delta x \, \Delta k = \pi \qquad [\because p = \hbar k.]$$

$$\Rightarrow \boxed{\Delta x \cdot \Delta p = \pi \hbar = h/2.}$$

- Recalling the Heisenberg uncertainty principles that $\Delta x \, \Delta p \geq h/2$ (which we have not yet discussed), we find that a Gaussian wave packet corresponds to equal uncertainty in both position and momentum space. The Gaussian wave packet has the least and equal uncertainty in both position and momentum space. On the contrary, the $\delta$ function wave packet has no uncertainty in position but infinite uncertainty in momentum. The plane wave

solution has no uncertainty in the momentum but infinite uncertainty in the position space.

- Generalizing the above analysis to any variable $(\theta, t)$ and its conjugate variable $(L, E)$, we can obtain the uncertainty relation:

$$\Delta E \, \Delta t \geq \hbar/2$$
$$\Delta L \, \Delta \theta \geq \hbar/2.$$

[ Then also the fact that $(x \& p)$, $(L \& \theta)$ have a Poisson bracket which we will convert to commutator as we will go to QM. Then the uncertainty relation is evidently related to the Poisson Bracket:

$$\Delta p \, \Delta x \geq \frac{1}{2} \langle \{p, x\} \rangle \geq -\frac{i}{2} \langle [p, x] \rangle. \; ]$$

- H.W. Consider $g(x) \sim e^{-(x-x_0)/\epsilon_0}$ and find $\langle x \rangle$ & $\Delta x$.

- H.W.: $P(k) = \int g(x) \, e^{-ikx} \, dx = \int \psi^*(x) \, \psi(x) \, e^{-ikx} \, dx$

$\psi$ F.T. $\int \frac{dq}{(2\pi)} \, \phi^*(q) \, e^{iqx}$

$\int \frac{dq'}{(2\pi)} \, \phi(q') \, e^{-iq'x}$

$= ?$

- Linear vector space and matrix Algebra:

  To be discussed before introducing matrix quantum mechanics. (Heisenberg Representation).

# History : Experimental Evidence of Quantization

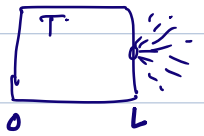
(A) Light is Particles.
(B) Atom have discrete orbits.
(C) Particles (Electrons) are wave.

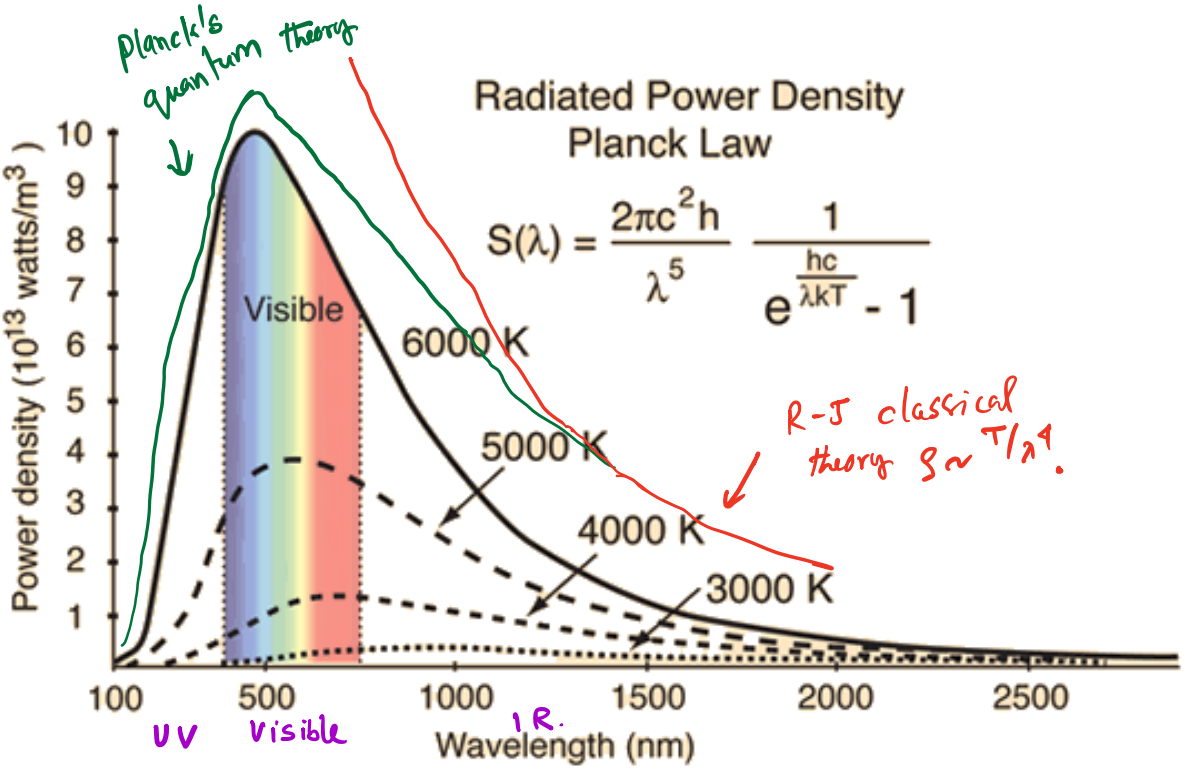
## (A1) Black Body Radiation :

Bransden (1.1)
Weenberg (1.1)

A back body is defined by a body which absorbs all the radiant energy falling upon it ie, its absorption coefficient is unity at all wavelength. Its emissive power (power emitted per unit area at a given wavelength) is same as its absorption power, ie, unity. The black body radiation is a universal (but idealized) property. G.R. Kirchhoff studied this property between 1859-1862 and gave the name black body radiation.

Quantum mechanics had its begining in the study of black body radiation. Consider an enclosure whose walls are kept at a temp. $T$, and suppose that the energy/volume of radiation lying in the wavelength range $\lambda$ to $\lambda + d\lambda$ is $S(\lambda, T)\, d\lambda$. The measured distributions of $S(\lambda, T)$ in the wavelength space is shown in the picture:






## Classical & Statistical & Electromagnetic Theory

- John W. Strutt followed by Lord Rayleigh & James Jeans between 1900-1905 wrote series of paper to reproduce the above distribution curve. The idea was that we have the wave equations that we saw before with plane wave solutions $e^{i(\vec{k}\cdot\vec{r} - \omega t)}$ where all wavenumber $k$ and frequencies $\omega$ are allowed in general. But now as we confine the electromagnetic radiation in a cavity (lets consider a cube of length $L$ for simplicity) the plane waves form standing waves. Now only those waves are allowed which follow the periodic boundary

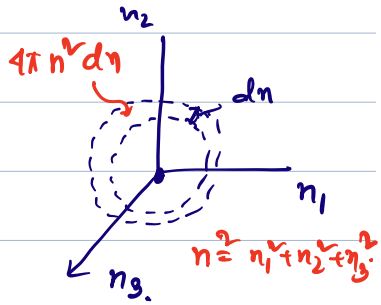
Condition that $e^{ikx} = e^{ik(x+L)}$ along all three directions. This gives $e^{ikL} = 1 \Rightarrow k = 2\pi n/L$ where $n$ is +ive integer. This gives a discrete spectrum of wavelength $\lambda = L/n$, and hence frequency $\nu = c/\lambda = cn/L$. But we assume $L \gg n$ that the spectrum is almost continuous. Then we just need to know how many such modes lie in the range $n$ to $n+dn$, i.e the density of wavelengths $N(\lambda)$ is defined as.

$$N(\lambda)\, d\lambda = 2 \times 4\pi n^2\, dn$$

(2 - possible polarization)

$$= 8\pi \frac{L^2}{\lambda^2}\left(\frac{L}{\lambda^2}\, d\lambda\right)$$

$$= \frac{8\pi L^3}{\lambda^4}\, d\lambda \quad \text{---(1)}$$




(Since the modes are excited equally along all three directions.)

So, $\boxed{N(\lambda) = \frac{8\pi}{\lambda^4}}$ (per unit volume $L^3 = 1$.)

- Now each mode carries energy $\boxed{\bar{E} = k_B T}$ as obtained from the equipartition principles ($\frac{1}{2} k_B T$ each for K.E & potential energy).
- Therefore, $\boxed{S(\lambda, T) = N\bar{E} = \frac{8\pi}{\lambda^4} k_B T}$ --- (1).

The Rayleigh-Jeans (R-J) result gives a good fitting to the experimental data at long-wavelength limit

which we will refer to the classical limit. But experiment shows a maximum peak in the visible frequency range for the studied temperature and then it drops to zero in the UV region and thus having no radiation. But the R-J formula rather diverges at $\lambda \to 0$ which is known as the "Ultraviolet catastrophe".

⊙ **Planck's quantum theory:**

While R-J obtained quantized wavelength & frequency (although the above calculation used its continuum limit, but the same result can be obtained by assuming discrete wavelength & frequencies). But they assumed continuous energy spectrum ($E = k_B T$). Although we gave a hand-waving argument from the least action principle that frequency & energy can be related to each other via a multiplicative factor of the dimension of the action, but during that time such a relation did not exist. Planck was the first person in 1900 to propose that for every discrete radiation mode, the energy is also quantized. The energy vs frequency relation was proposed by Planck was

$$\boxed{E = h\nu = \frac{hc}{\lambda}} \quad \cdots (2)$$

where $h$ = universal constant called Planck's constant and has the dimension of the action (i.e., $[h] = [S] \sim [E][t] = [P][x] = [L][\theta]$ ---). The value of $h$ that we know now is $h = 6.62618 \times 10^{-34}$ J.S.

Then the average energy per mode can be deduced is

$$\bar{E} = \frac{\sum_{n=0}^{\infty} E_n e^{-\beta E_n}}{\sum_{n=0}^{\infty} e^{-\beta E_n} = Z}$$

$\beta = 1/k_B T$.

$E_n = \frac{hc}{L} n = n\epsilon_0$.

$\epsilon_0 = \frac{hc}{L}$.

$$= -\frac{d}{d\beta} \log Z$$

$$\boxed{\bar{E} = \frac{\epsilon_0}{e^{\beta\epsilon_0} - 1}} \quad --(2)$$

$Z$ = Partition function

$$= \sum_{n=0}^{\infty} e^{-\beta n \epsilon_0}$$

$$= \frac{-1}{e^{-\beta\epsilon_0} - 1}$$

Then we get

$$\boxed{S(\lambda, T) = N(\lambda)\bar{E} = \frac{8\pi hc}{\lambda^5} \frac{1}{e^{hc/\lambda k_B T} - 1}} \quad --(1).$$

- This formula in eq (1) matches very well with the experiments in all wavelength regions.
- Note that the R-J classical theory matches well at

long-wavelength limit. Show that the Planck's quantum theory reaches to classical limit as $\lambda \to \infty$. In fact Bohr proposed that whatever quantum theory one obtains should reproduce the classical theory as $h \to 0$. This is called the Correspondence Principle.

- The physical reason behind it as follows. The energy separation between the discrete energy level is $hc/L \sim hc/\lambda$. Therefore, as $h \to 0$, or $\lambda \to \infty$, one approaches towards the continuum of energy levels and one approaches towards the classical regime.

- At a given temperature T, the approximate thermal energy is $k_B T$. Therefore, a quantum regime is reached when $k_B T < h\nu = hc/\lambda$ such that the thermal fluctuation is less than the discrete energy levels. As $k_B T >> hc/\lambda$, the thermal fluctuation smears out the distinct energy levels and one obtains classical limit. The peak in $\mathcal{E}(\lambda, T)$ corresponding to the transition from quantum to classical regime is roughly obtained at.

$$k_B T \sim hc/\lambda.$$

[ H.W. Compute Radiation pressure & Specific heat of the Black body Radiation. ]

- Planck's proposal of quantization of energy was ad-hoc and was not accepted easily. But the idea was correct and with the development of modern quantum theory we have verified the quantization of energy.

- In the above black body radiation theory, the source of quantization of the radiation was the periodic boundary condition due to confinement in a cavity. Then Planck proposed a linear relation between energy & frequency. Since wavelength & frequency is quantized due to periodic boundary condition, and hence energy is quantized.

- In contrast, Einstein proposed in 1905, to explain Photo electric effect that light, i.e, the plane wave solutions of the wave equation is always quantized even in a free space without confinement. Therefore, even a plane wave solution of light does not take continuous values of $k$, $\nu$, but discrete values of $k$, $\nu$ and hence energy. He did not derive any relation but only used Planck's proposal of $E = h\nu$ but used discrete values of $\nu$ even in free space to explain the photo electric effect. The minimum

value of $\nu$, denoting as $\nu_0$, is the most fundamental frequency. They called it corpuscles or quanta of light which was later renamed as photon. This is like a fundamental / elementary relativistic particle of energy $E = h\nu_0$ but no rest mass.

George Gamow later remarked that radiation is like butter, because, even though butter itself comes in any quantity but it can be bought & sold only in multiples of one quarter pound.

## (A2) Photoelectric effect :

Fig 2a

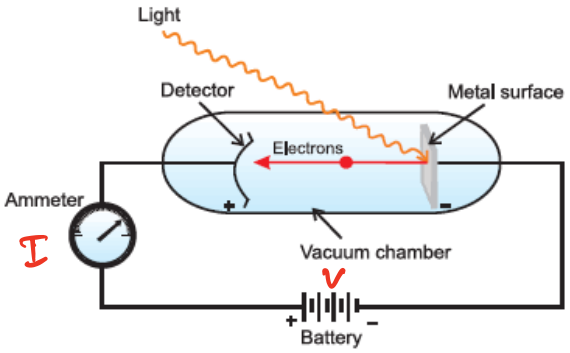



Fig 2b

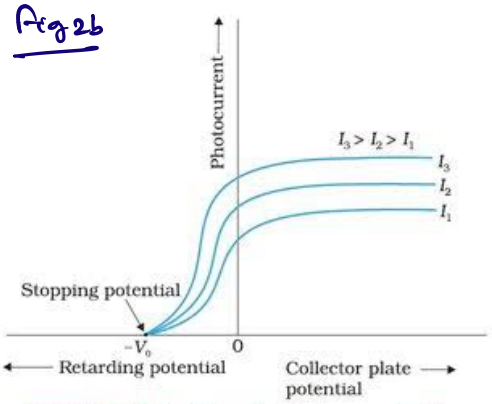
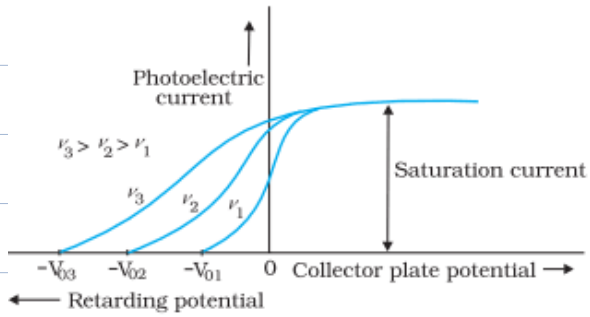



FIGURE 11.3 Variation of photocurrent with collector plate potential for different intensity of incident radiation.

Fig 2c




Hertz in 1887 and Lenard in 1900 used the setup shown in Fig (2a). They found that charge particles (which we later know to be electrons) are emitted from metal surface when radiated with high-frequency (UV range) lights. This phenomena is called the photo-electric effect. The emitted electrons from the photocathod is collected at the anode plate, and a circuit is completed to measure the current (I). In addition, a battery is added to maintain

a voltage (V) difference between the cathod and anode. The voltage difference is given in reverse direction to repel the electron ejected from photocathode, so that only electrons with higher kinectic energy can reach the anode. Therefore, only those electrons whose K.E. is higher than eV (e = charge of electron) will reach the anode. As $V < 0$ is increased in magnitude, less and less electron reach the anode and then it stops at a voltage $-V_0$. This is called the stopping voltage (see fig 2b). So, the maximum K.E of the emitted electron is

$$E_{max} = \frac{1}{2} m v_{max}^2 = eV \quad - (1).$$

Observations

(i) It was surprisingly found that the stopping energy is independent of the intensity of light. From classical wave theory, we expect that the energy of light is proportional to its intensity and more energy of light means more K.E. of ejected electron. But the result says, the K.E. of photoelectron is independent of the intensity of light. Higher light intensity only ejects more electrons of same energy. (We are only focussing on highest K.E. electron which presumably resided on the surface. The other lower energy electrons come from inside the material).

(ii) On the contrary, as shown in Fig 2c, as the frequency ($\nu$) of the light is changed with the same intensity, the stopping potential ($-V_0$) changes linearly with $\nu$, but the saturated current remains the same. (There is a threshold frequency $\nu_t$ below which no photoelectron is ejected, irrespective of intensity & long-time exposure of light).

So,

(a) The (highest) K.E of photoelectron $E_{max} \propto \nu$ (freq of light)

(b) The # of photoelectron $\propto$ Intensity of light.

[ According to classical wave theory: (i) photoelectric effect should occur for any frequency of light, provided its intensity is large enough and the exposure time is long enough to provide sufficient energy to eject an electron ].

- Einstein generalized Planck's idea of energy quantization in a blackbody cavity to the quantization of energy of electromagnetic plane waves even in free space:

$$E = h\nu = hc/\lambda \quad \text{--- (1)}$$

where the discrete frequencies $\nu$ are integer multiple of some minimum frequency $\nu_0$ as

$$\nu = n\nu_0 \quad \text{--- (2)}$$

The origin of the minimum energy $\nu_0$ and the other quantum number $n$ was not provided by Einstein, but he argued that light is made of particles with each particle carries an energy $h\nu_0$. These particles have no rest mass. These particles are called "photon".

- Although the photoelectric effect provides a compelling evidence of the corpuscular theory of light, it must not be forgotten that the existence of diffraction / interference phenomena demonstrate the wave nature of light. This dual nature of light (which we shall see soon for electron also) is incompatible with classical theory.

## (A 3) Compton Effect:

After the discovery of X-ray by W. K. Röntgen in 1895, a revolution in the interaction between light & electron in matter become possible. Because X-ray wavelength ~ Å same order of atomic radius..

Fig 3a

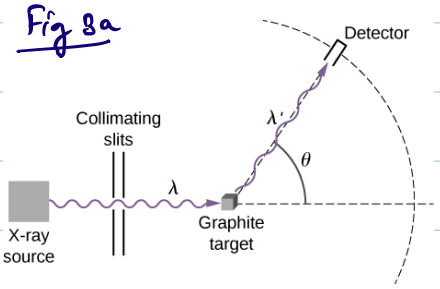
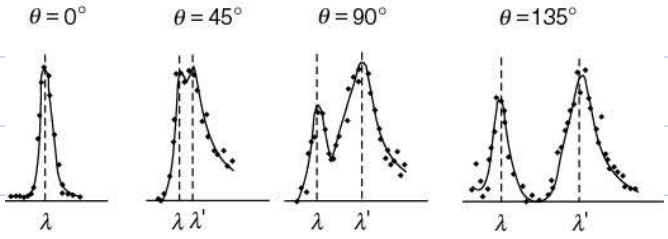



Fig 3b




Unlike the photoelectric effect of light-in, electron-out, Compton made a measurement setup to have light-in and light-out after scattering with atoms / electron in graphite. The incident light has a fixed wavelength of $\lambda$, the outgoing light has two peaks, one at $\lambda$ and another at $\lambda' > \lambda$. The splitting between the two peaks become sharp with increasing detector angle, as shown in Fig 3b.

- According to classical wave theory of light, the incident plane wave will be incident on rest electrons. The electron will then start oscillating with the same frequency and therefore radiate back the electromagnetic wave at the same frequency. So, the wave theory will explain the presence of a peak at

the incident wavelength $\lambda$. The second peak cannot be explained by the wave theory.

- Taking clue from the fact that the wavelength of the second peak depends on angle $\theta$, Compton thought about the similarity with scattering between two particles. By this time Einstein's two papers on light as photon and particle at the speed of light follows relativistic relation were already published. Compton considered photon as relativistic particle whose energy is $E = \sqrt{p^2c^2 + m^2c^4}$, with its rest mass $m = 0$. So, $E = pc$. Then the energy is quantised to $E = h\nu$. So, $\boxed{p = \frac{h\nu}{c} = \frac{h}{\lambda}}$ ---(1).

which gives a relation between wavelength with the momentum of a particle which will be equivalent to the de Broglie wavelength $\lambda$ of a particle like electron. Then using momentum and energy conservation at the scattering between photon and electron, one easily obtain the relation

$$\boxed{\lambda' - \lambda = \frac{h}{mc}(1 - \cos\theta).} \quad \text{---(2)}.$$

The existance of the unmodified wavelength $\lambda$ is due to the scattering of the light with core electrons tightly bound to atoms.

(H.W.) Derive eqn (2).

## Heisenberg Microscope (Hypothetical) and an invitation to his uncertainty principle.

The Compton effect was possible due to the discovery of X-ray because X-ray has high frequency and wavelength which are in the same order of magnitude of electrons' energy in atom and the radium of atoms or interatomic distance in solid ($\sim$ Å). Visible light has frequency smaller than even the loosely board electrons and thus only shows one wavelength peak at $\lambda$. On the other hand, $\gamma$-ray only show the shifted peak at $\lambda'$ because its energy is very large compared to the core electron's energy.

The relation between p & $\lambda$ in eq(5) and the inability to scatter the free electron at any wavelength gives an hypothetical intuition to the inability to measure both p & position of a particle simultaneously with arbitrary precision. (Although the uncertainty principle is more fundamental to the quantum theory as discussed briefly above, and has nothing to do whether the measurement is done with a certain wavelength of light or not, but many books discuss it as if the measurement is done with light. Some people also refer to it as Heisenberg Microscope.)

The relation $p = h/\lambda$ seems to impose a restriction on the simultaneous measurement $p$ & $x$ of a particle, atleast if the measurement is done with light. The argument is as follows. To measure the particle at a position $x$ with its accuracy $\Delta x$, we need a light of wavelength $\lambda < \Delta x$. But the photon at this wavelength $\lambda$ carries momenta $p = h/\lambda$ which, during the measurement, is transfered to the particle. So, now the particle's momentum has changed by $\Delta p \sim h/\Delta x$. So, the order of magnitude calculation gives

$\Delta x \, \Delta p \sim h$, the lower bound on uncertainty.

(A 4) Raman Effect (1928): While compton scattering is elastic scattering between photon and electron, Raman also observed the presence of inelastic scattering (with reduced intensity of outgoing light). In Raman scattering mechanics the outgoing light has different energy than the incident light in which the photon gains or looses energy to the atom/molecule. It was explained subsequently that the balanced energy (and also momentum in some cases) are absorbed/emitted by the vibration of the atom/molecule. This means, not only electromagnetic waves but the vibrational waves (like sound wave) is also quantized, called phonons. We will solve this problem in great details that the atomic vibrations which are like balls attached by spring have discrete set of frequencies and energy and this is one of the easiest but most fundamental building blocks of quantum mechanics.

H.W. Assuming $E = (n+1/2)h\nu$ for vibrational spectrum, obtain the $S(\lambda, T)$ vs $\lambda$ relation and the specific heat of this system.

## (B). Atomic Spectra and the Bohr model of Hydrogen atom.

As early as 1725, T. Melvill and subsequently many others showed that the emission and absorption line spectra of atoms are same and discrete. They are called emission lines. By the work of Balmer in 1885, followed by Rydberg in 1889 and so on, it was realized these emission/absorption lines have a regular pattern, as seen in Fig 4a.

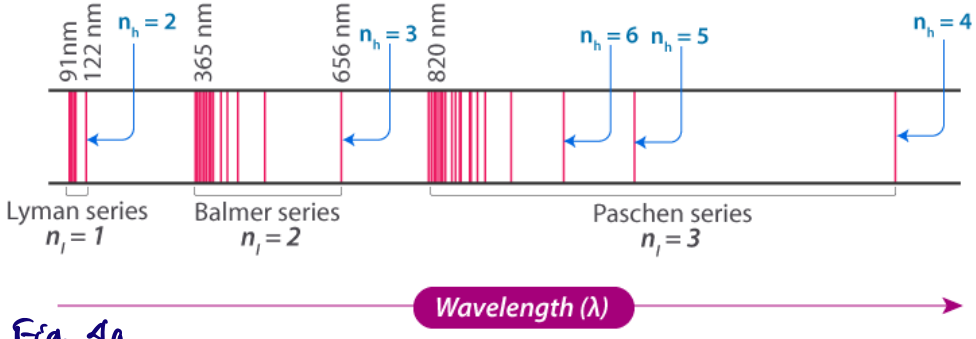



Fig 4a

All these lines can be reproduced by Balmer-Rydberg formula

$$\frac{1}{\lambda_{ab}} = R_H \left( \frac{1}{n_a^2} - \frac{1}{n_b^2} \right) \quad --(1)$$

where $R_H$ = Rydberg constant = $109677.58\ cm^{-1}$.

$n_a = 1, 2, \ldots$

$n_b = 2, 3, \ldots$

and $\lambda_{ab}$ is the wavelength of either emission or absorption lines.

The existence of atomic line spectra, as shown in Fig 4a, which exhibit regularities, cannot be explained by models of atomic structure based on classical physics. Neils Bohr in 1913 proposed the idea of quantized circular orbit with quantized energy in hydrogen atom to explain the above phenomena is considered an introduction to quantum theory for electrons.

The model of Nucleaus: During this time, Rutherford in 1911 showed by scattering of atoms through alpha particle ($He^{2+}$) that atom is mostly empty. Its all the positive charge and almost all its mass is concentrated in the nucleus ($\sim 10^{-14}$ m), which is much smaller than the atomic size ($\sim 10^{-10}$ m). (In 1911, Geiger & Marsden reproduced this observations). Then the electrons are circulating around the nucleus like a planetary motion by virtue of the Coulomb attraction. But unlike stable planetary motion of neutral particle, the rotation of charge particle in a closed loop is accelerating and hence the produced magnetic field at the center is time-dependent. From Maxwell's equations, we saw that this will produce electromagnetic wave which will take away the energy. Therefore, electron will energy and eventually fall back to the nucleus. So, atom will not be stable.

## Bohr's model of Hydrogen Atom:

To explain the above discrete atomic spectrum and Rutherford's observation of orbital motion of electrons, Bohr in 1913, used the idea of Planck's & Einstein's model of quantized energy, in each orbit. Bohr proposed that the energy of electrons in an orbit is quantized. Unlike Planck & Einstein, Bohr did not start with an assumption that energy is quantized, but rather he started with an assumption that orbital angular momentum in a circular motion is quantized. From there, he derived how energy is quantized.

[ We can rederive the Bohr's quantization formula starting from the classical mechanics' least action principle and the Bohr-Sommerfeld's quantization condition. Recall from the Noether's theorem that if the system is rotationally invariant, then the orbital angular momentum $L$ is conserved. We just have to show that the angular momentum is conserved not to any value but only discrete values of $\hbar$. As we often write an action in $x, p$ phase space coordinates (which are conjugate to each other and $p$ is the conserved quantity of translational symmetry), for the same argument, one can as well write the theory in the polar coordinates and its conjugate variables. Assuming

that the motion is fixed circle, ie, we can assume the motion in fixed on a constant radius (in any dimension). Then in 3D, the motion is described described by three Euler angles $(\theta_x, \theta_y, \theta_z)$ for rotations w.r.t. x, y, z axes. The corresponding conserved conjugate variables are $L_x, L_y, L_z$. (In reality having the motion constraint on a constant radius sphere, the three independent variables reduces to a two independent angles. This also makes among $L_x, L_y, L_z$, only two are related to each other. Their relation is denoted by a commutator in QM : $[L_x, L_y] = iL_z$, and its cyclic relation. We will here ignore this complication and only assume a 2D circular motion denoted by $\theta$ and the corresponding angular momentum is $L$.).

Then via analogy we can write the action as

$$S = \int dt \left[ L\dot{\theta} - H(\theta, L) \right] \quad \text{---(1)}$$

and the Bohr-Sommerfeld quantization in the corresponding phase space of $(L, \theta)$ as

$$\oint L \, d\theta = nh \quad \text{--- (2)}$$

[ Compare with $S = \int dt [p\dot{x} - H(x,p)]$ & $\oint p\,dx = nh$ ].

Then assuming $H$ & $L$ being conserved (i.e, $\dot{L} = \{H, L\} = 0$) we obtain

$$\oint H\, dt = \oint L\, \dot{\theta}\, dt = \oint L\, d\theta$$
$$= L \oint d\theta = L\, 2\pi$$
$$\Rightarrow \boxed{L = n\hbar} \quad \text{---(3)} \qquad (\hbar = h/2\pi)$$

& $H \oint dt = HT = nh$ where $T$ = time period
---(4).

We now need to compute $T$.

Since Coulomb force is the only force giving the centripetal acceleration $v^2/r$, we obtain $\frac{Ze^2}{4\pi\epsilon_0 r^2} = \frac{mv^2}{r}$ —(5).

From eq (3) $L = mvr = n\hbar$ --(6)

Using eq (5) & (6), we get $v = \frac{Ze^2}{4\pi\epsilon_0}\frac{1}{\hbar n}$ , $r = \frac{4\pi\epsilon_0}{Ze^2 m}\hbar^2 n^2$.

Then the time period is $T = \frac{2\pi r}{v} = 2\pi\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2 \frac{1}{m}\hbar^3 n^3$.

Then from eq (4) we get

$$\boxed{H = E = -\frac{m}{2\hbar^2}\underbrace{\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2}_{R_H}\frac{1}{n^2}} \quad , \quad n = 1, 2, 3 \cdots \infty$$
---(7).

Remember that the integer $n$ in the Bohr's theory has no proper justification. It's the orbital angular momentum of

each orbit. This is called the principle quantum number. Eq (7) reproduces the Balmer - Rutherford formula and gives a very good estimate of the Rutherford constant $R_H$. The correction from circular to elliptic orbit gave a better agreement to the value of $R_H$.

- The Bohr Correspondence Principle: Bohr proposed that a quantum theory can be considered a valid theory if one can take it to the classical limit by taking $h \to 0$ and/or the energy separation between the discrete levels is small (compared to some other energy scale like $k_B T$) which should reproduce the classical result.

  (H.W. By taking $n \to \infty$ limit show that the Bohr's result reproduces the result of a classical orbit.).

# Bohr-Sommerfeld Quantization Condition

It was actually Sommerfeld in 1916, derived the quantization condition in which he generalized the Bohr's quantization condition for circular orbit to an elliptic orbit in which the energies are quantized. Sommerfeld's condition was that in a system described by a Hamiltonian $H(p, x)$ with several coordinates $x_i$ & canonical conjugates $p_i$ satisfying the Hamilton's equations $\dot{x}_i = \partial H/\partial p_i$ ; $\dot{p}_i = -\partial H/\partial x_i$, if all $x_i$ & $p_i$ have a periodic time dependence (as for a closed orbits), then for each $i$, we have

$$\oint p_i \, dx_i = n_i h \quad , \text{ with } n_i \in \mathbb{Z} \text{ (integers).}$$

The integral is taken over one period of the motion.

This relation generalizes to any general coordinate, e.g. $\theta_i$ and its conjugate variable $L_i$ as

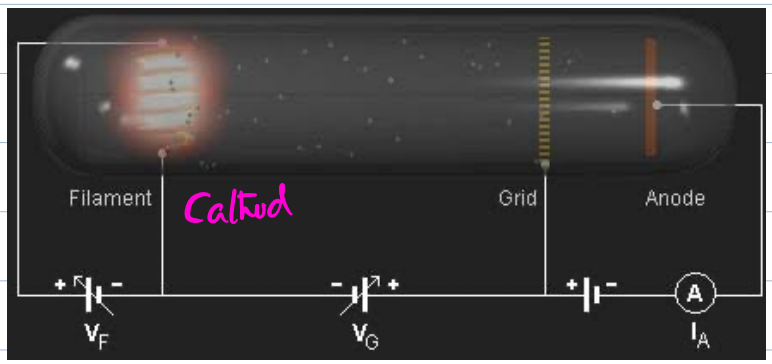
$$\oint L_i \, d\theta_i = n_i h.$$

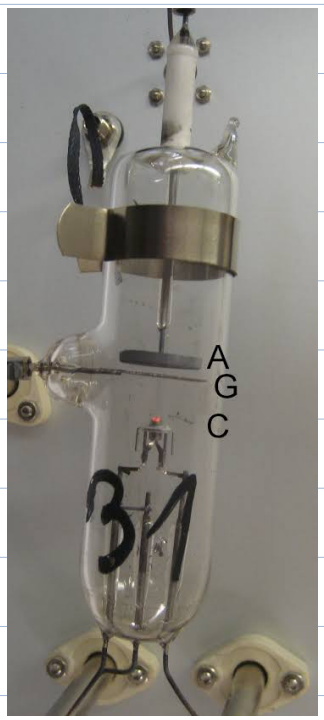
As we also argued that the least action principle dictates that the energy, time quantization condition is hence obtained as

$$\int_0^T H(x_i, p_i) \, dt = n h.$$

(This approach is limited and only applies to periodic motion, whereas quantum theory is general to all trajectories).

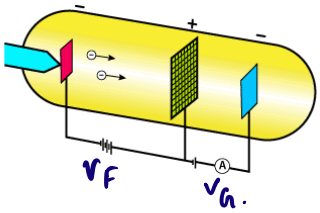
- **Franck-Hertz Experiment:** Measurement of energy quantization of atoms with out light



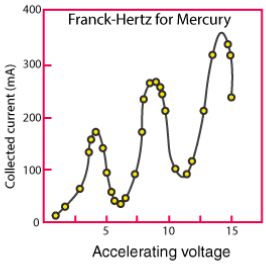




**FRANCK - HERTZ EXPERIMENT**

BYJU'S The Learning App




Accelerating apparatus

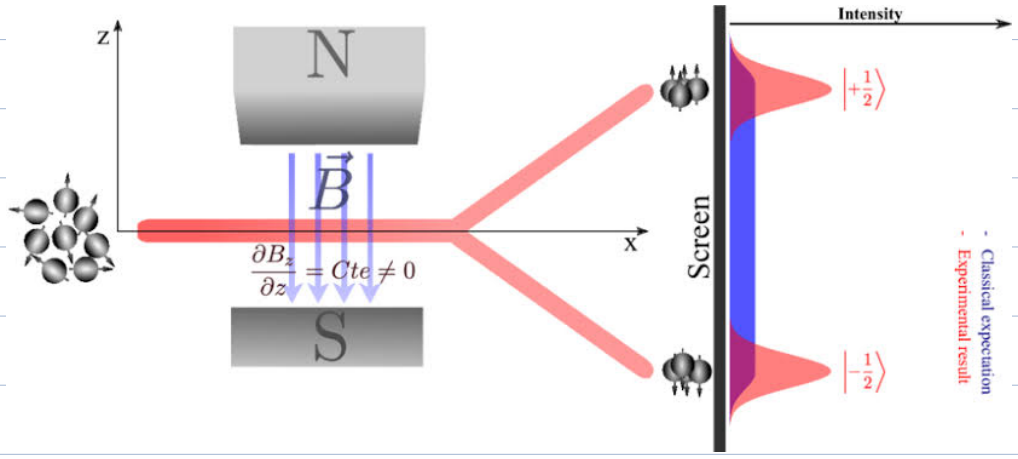



In 1914, J. Franck and G. Hertz directly measured the energy quantization of atoms without using light. Therefore, it was proved that the quantization of atomic orbits has nothing to do with the quantization of light.

In an evacuated tube, electrons are ejected from a heated cathod and accelerated towards a wire grid, maintained at a positive potential $V_F$ w.r.to the cathod. The electrons gain K.E. $\frac{1}{2}mv^2 = eV_F$. The electrons are then collected by a plate, causing a current I. The collecting plate is maintained at a potential $V_G$ ($V_G \leq V_F$), the accelerating voltage $\Delta V = V_F - V_G$. The tube is

then filled with mercury gas. The accelerated electron collide elastically with the mercury atom, because mercury is heavy. But when the electrons' energy ($\Delta V$) matches exactly with an orbital energy of the Hg-atom, it can loose its energy to the Hg atoms via elastic scattering. The observed current vs voltage profile shows dips at the energy intervals which matches with the atomic energy levels predicted by Bohr for Hg.

## Stern - Gerlach Experiment: Measurement of angular momentum quantization and the discovery of Spin.




O. Stern & W. Gerlach in 1922, made an experimental setup to verify the quantization of angular momentum that Bohr proposed. The orbital angular momentum of electron is like a magnetic dipole (magnet because it is the charge particle which is rotating in a circle producing a magnetic field at the center. The orbital magnetic moment

$$\vec{M} = -\frac{e}{2m}\vec{L} \quad \text{where} \quad \vec{L} = \vec{r} \times \vec{p}.$$

of a magnetic dipole $\vec{M}$ is placed under a magnetic field $\vec{B}$, the potential energy due to the interaction is $U = -\vec{M} \cdot \vec{B}$.

The torque $\vec{T} = \vec{M} \times \vec{B}$, and a net force is $\vec{F} = -\vec{\nabla} U$.

Due to variation of the magnetic field, the force is acquired to be $F_i = \vec{M} \cdot \frac{d\vec{B}}{dr_i}$, $i = x, y, z$. For an uniform magnetic field, there is however no force since $\vec{M}$ is uniform. Then the

magnetic dipole precesses with a constant angular frequency $\omega_L = \frac{\mu B}{\hbar} B$, called Larmor angular frequency. With inhomogeneous magnetic field, the atoms can be defected due to its magnetic moment and hence we can measure $\vec{M}$.

With this principle, Stern & Gerlach in 1921 build the above setup to pass beams of electrons through an inhomogeneous magnetic field. In the incident beam, the direction of the magnetic moment $\vec{M}$ of electrons is random and along the $z$-direction, one would obtain value in the range $-M \leq M_z \leq M$. So, in the detecting plate the atoms would spread over continuously. The surprising result that Stern & Gerlach obtained, as shown in fig above, that <u>two distinct</u>, separate and <u>symmetric</u> around zero deflection line are present. The same result was obtained in many elements. According to Bohr's model, $L = n\hbar$, where $n = 0, 1, 2, \cdots$. The maximum value of $L_z = +n\hbar$ and its minimum value is $-n\hbar$, i.e. $L_z = n\hbar$, where $m = -l, -l+1, \cdots 0, \cdots l$, taking $(2l+1)$ values. Therefore, one would expect $(2l+1)$ spots in Stern-Gerlach experiments. But what they rather found two spots which corresponds to $l = 1/2$, not even integer.

In 1925, S. Goudsmit and G.E. Uhlenbeck analyzed the splitting of atomic spectral lines occuring in a magnetic field (Zeeman effect). They proposed that the splitting of the spectral lines into two can be explained if the electrons possess intrinsic angular momentum, ie, spin. With analogy to the relation between $\vec{M}$ & $\vec{L}$, one writes expresses the internal magnetic momentum into a spin angular momentum as

$$\vec{S} = -\hbar \vec{M}_S / g_S \mu_B \text{ , where}$$

$\mu_B = \frac{e\hbar}{2m}$ is the Bohr magnetic, and $g_S$ is a proportionality constant, called gyromagnetic ratio, to fix the value of $S_z = \pm 1/2$ as seen in Stern-Gerlach experiment. Therefore, the total angular momentum of spin is

$$\boxed{\vec{M} = -\frac{\mu_B}{\hbar}\left(\vec{L} + g_S \vec{S}\right)}.$$

The quantization of the spin of the electron to 1/2 (so that it explains the two peaks feature within the formula of $(2S+1)$ multiplicity) has no explanation from classical mechanics and is a purely quantum mechanical effect. In fact, no one knows its origin, but the consequence of having 1/2 spin and 2-fold multiplicity has important quantum mechanical consequence, that distinguishes electron from photon / phonon and are called fermions.

## (C) Electrons are waves

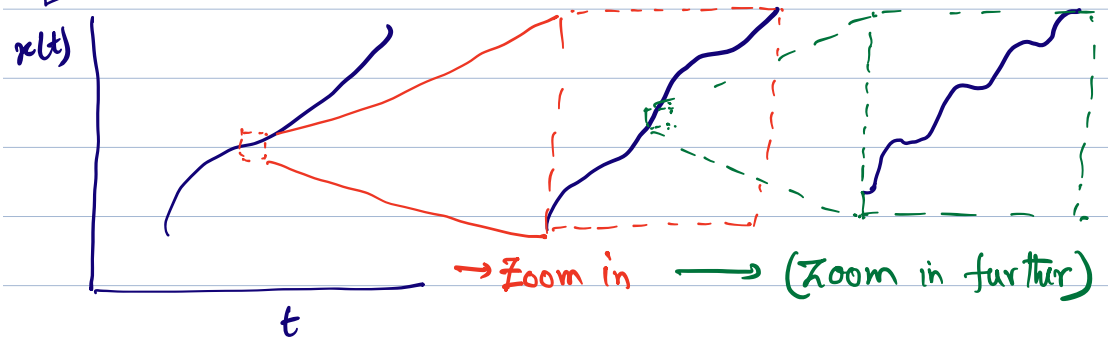
So far we have been collecting evidence of light behaving like a particle with a quanta of energy $h\nu_0$ and momentum $p = h/\lambda = \frac{h\nu}{c}$. We have also seen from black-body radiation that the particle like (quantum mechanical) behavior is appreciable as we go to the high frequency (UV) and short wavelength limit. There is no hard and fast rule of when a quantum mechanical scale appears. It's all depends on the other energy and length scales of our system / measurements. For example, the discrete energy spacing $h\nu_0$ should be large enough compared to the energy resolution of the instrument or larger than the thermal fluctuation $k_B T$, so that we can probe the discrete energy levels. Similarly, the wavelength $\lambda$ should the small enough ($\sim h$) to be able to probe the momentum of the particle with high accuracy. Otherwise the particles are moving very fast and the error in measurement $\Delta p$ can be very large and then $\Delta p \Delta x \gg h$, and hence we are far from the quantum limit.

(An analogy would be a fan. When a fan rotates on high speed, we don't see its discrete blades. But at low speed we see them).

## De-Broglie Hypothesis:

It turns out, the reverse is also true. What we call a particle in classical physics also behaves as wave if we go to the length scale $\sim 10^{-10}$ m. Because, the waves are very short-wave lengths ($\sim 10^{-10}$ m) and very high frequency. Therefore, unless we have a right experimental setup with light with small wavelength (comparable to the wavelength of the particle, or that we are not at sufficiently low temperature such that the thermal energy $k_B T$ is comparable or less than the energy separation between the discrete energy levels we don't see them. Bohr & Sommerfeld's proposal of quantization of electron's energy and angular momentum in a periodic motion. But such a quantization and wave nature exists for all particles, just its wavelength is very short and frequency is very high. This is shown as in the fig. below.

$[p = h/\lambda]$




Any classical trajectory → zoom into to lengthscale $\sim 10^{-10}$ m.
→ Wave nature is visible.

- The above schematic figure illustrate this process. We take any arbitrary classical trajectory and zoom into the length scale $\sim 10^{-10}$ m, we will find an oscillatory nature of the trajectory. The above illustration is only for a periodic behavior of $x$ in $t$ as $x(t) \sim e^{i\omega t}$, where $\omega$ is very very fast causing rapid oscillation of the particle. The corresponding wavelength is defined in the position is also small. But to define a proper wavelength we need a function $\psi(x,t)$ to denote the trajectory both in space & time - that's a reason we adopt wave function description of the trajectory.

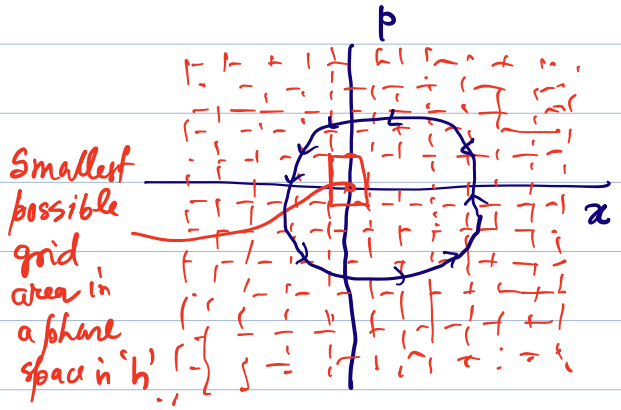
- Before we discuss the origin of this underlying wave nature of all trajectories, let us comment on the possible values of the wavelengths. As we said earlier, any continuous (also some discrete), differentiable function $\psi(r,t)$ can be expanded in the plane wave basis $e^{i(\vec{k}\cdot\vec{r} - \omega t)}$ with proper coefficients $\phi(k,\omega)$. The coefficients carry the information about the weight / probability / contributions from each plane wave components of wavenumber $k = 2\pi/\lambda$. It is obvious that smoother the function $\psi(x,t)$ in space $x$, lesser the contributions from higher wavelengths $\lambda$ are. A completely oscillatory classical path (like a Harmonic oscillator) has a well defined wavelength, so a wave nature is evident. On the contrary, a completely localized particle

(a delta function wave function) has equal contributions from all wave lengths.

- What's the origin of the underlying wave nature of the particle's trajectories. Although mathematically it makes perfect sense due to the Fourier transformation of "any" function (All equations of motions which are translationally invariant can have Fourier transformation), but its physical origin is not completely known. We can however discuss what's the physical implications of the underlying wave nature of particles.

We know that the particles trajectories are fully defined in a phase space. But then in a phase space, the degrees of freedom $p$ & $x$ are not completely independent (unlike linearly independent position variables), but they are related to each other by the Poisson bracket. You may think of it as every time we make an infinitesimal change in $x$, there is a change in $p$ contraints by the Poisson bracket (unless $p$ is a conserved quantity in which case the translation in $x$ is generated by the momentum only). The change is in such a way that after certain time and position, the trajectory make a rotation in the phase space about an area "$h$", or covers "$nh$" area in the

phase space. In other words the phase space can not be shrink arbitrarily to zero area, there is a minimum area of the phase space which is $\sim h$. So, the phase space is discrete, such that the wavelength of the Fourier modes cannot taken all the way to zero. In principle we should be doing a discrete Fourier transformations by considering all the discrete wavelengths separated by $\lambda \sim h/p$. Therefore, the shortest wavelength possible for a particle with momentum $p$ is




$$\boxed{\lambda = h/p} \quad --(1)$$

This is the de-Broglie wavelength which measures the distance the particle travels with momentum for it to sweep one bit of phase space area $\sim h$. The corresponding frequency is $\nu = \frac{1}{T} = \frac{p}{m\lambda}$. The quantum of energy is $E = h\nu = p^2/2m$ for non relativistic particles (for relativistic particle we have choose $E = pc = h\nu$ where $c = \lambda\nu$). This condition also makes the trajectory in E vs t "phase space" discrete as $\int_0^T E\,dt = ET = h$.

- The discrete nature of the phase space also puts restrictions on how the derivatives in the Hamiltonian principles are defined. $\dot{x} = \frac{\partial H}{\partial p}$, $\dot{p} = -\frac{\partial H}{\partial x}$. The derivative rule says

$$\frac{\partial H}{\partial p} = \lim_{\Delta p \to 0} \frac{H(p + \Delta p) - H(p)}{\Delta p}.$$

But the fact that both limits $\Delta p$ & $\Delta x$ cannot be taken simultaneously to zero, rather their limits have to be restricted to the minimum area of $\Delta p \, \Delta x \sim h$.

**Double slit Experiment:** Can we measure the wave nature of a particle trajectory?

**Ans:** Of course. We have to build a setup which will be sensitive to the wavelength $\lambda \sim h/p$ and then the interference and diffraction patterns are observables. So, we construct the double slit experiment with slit size $d \sim \lambda = h/p$, in analogy with Mach-Zehnder interferometer used for light.

- For the case of a plane wave of light, when coherent light is shined on a double slit as shown here, the plane-wave splits into two and then they start interfering with each other and produce an alternating bright and dark patterns on the screen. We have done this experiment with light and also showed that such a behaviour can only be explained by the wave nature of the light which is describle by a complex function having an amplitude and phase. At the two slits, the wave has split into two with equal amplitude but acquire

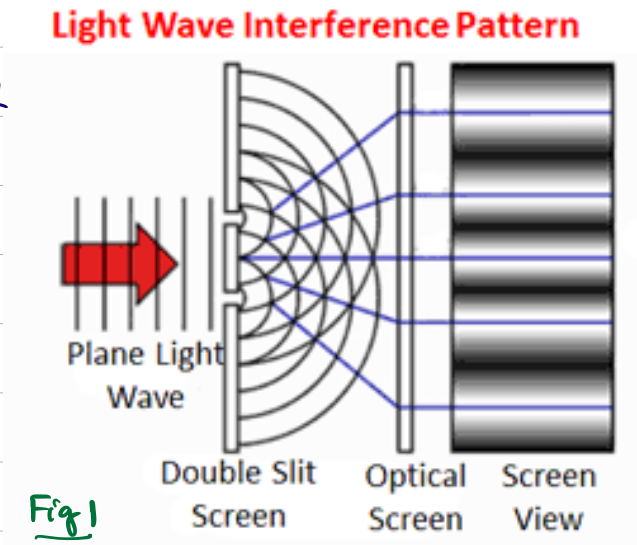
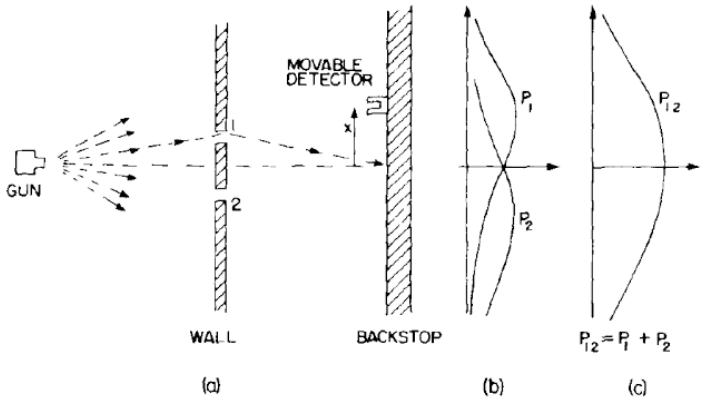


Fig 1

different phases determined by the path defferences between the two light rays.

Let us imagine doing the same experiment with particles with equal momenta turned with the slit sized such that $pd \sim h$.

Fig 2 : Classical picture



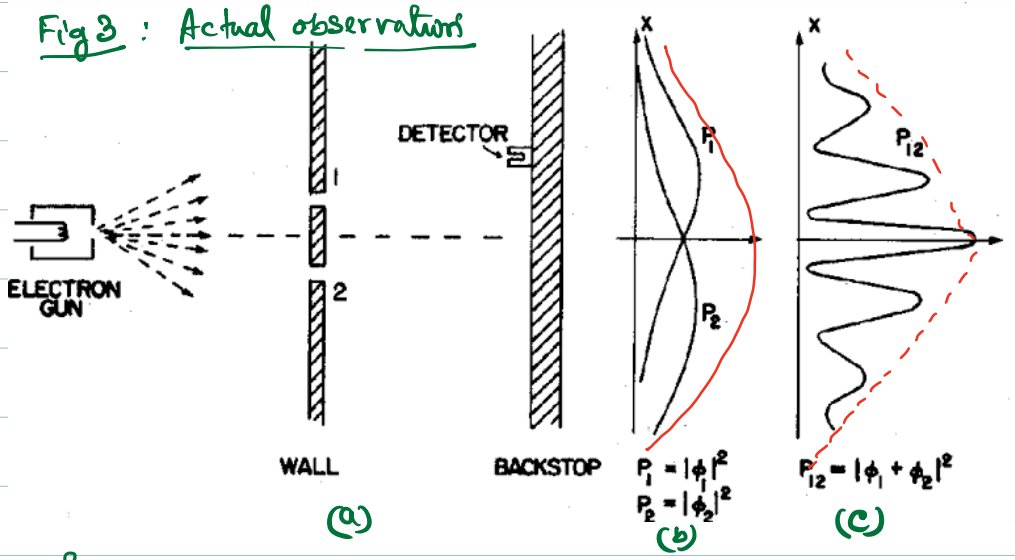

Classical picture (expectation from classical physics but not observed).

Let us first discuss what do we expect if the particles are not wave. Then the particle can either go through the slit 1 with a probability $P_1$ or the probability of going through slit 2 is $P_2$. (Without any bias, $P_1 = P_2$, but we keep them different for generality). Then each probability distribution (most likely will be gaussian) will have the shape as shown in Fig 2(b). Then the total probability (intensity distribution of particles collected by the detector) will be

$$P_{12} = P_1 + P_2 \quad \text{--- (1).}$$

as shown in Fig 2 (c).

Fig 3 : Actual observations




## Observation and Quantum Mechanics!

But what one observes is an ~~interference~~ pattern as shown in Fig 3 (c). The observed feature cannot be explained by simply adding the probability of passing through each slit, but by adding the complex waves $\phi_1$ & $\phi_2$ from the two slits $\phi_1 + \phi_2$ and then taking its amplitude $|\phi_1 + \phi_2|^2$. This is the same theory we need for light to explain its diffraction. So particles to trajectories are made of many many short-wavelength waves.

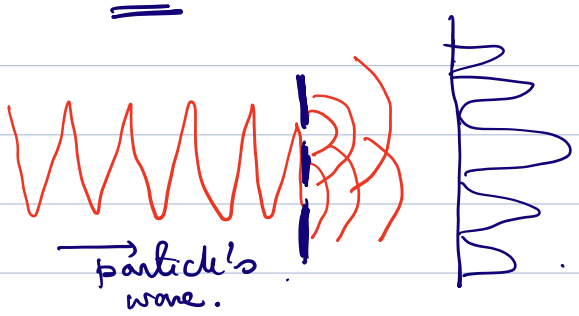
- If we use two detectors, one only detects particles from 1 & other from 2, we will observe Fig 3 (b). But a single detector will observe Fig 3 (c).

**Diffraction vs Interference:** Are we observing the interference patters of two different waves associated with two different particles (electron or photon) or are we observing the diffraction patterns of a single wave (a single electron or photon) which split by the two slits and then diffracts due to the phase difference?

Ans: If it was interference we will see Fig 3(b). For diffraction we see Fig 3(c).

- To verify it, we have to keep reducing the intensity of the incident particle until at any instant of time, there is only one particle coming out and going through "both" slits and then being detected. Then the 2nd particle is fired from the source. (This was demonstrated originally in 1909 by G.I. Taylor, who photographed the diffraction pattern formed by the shadow of a needle, using a very weak source such that the exposures lasted for months. It can be concluded that interference between two distinct particles wave' do not happen, but a property of a single particle. More recently in 1989, this experiment was confirmed by A. Aspect, P. Grangier and G. Roger for photon and for electrons by A. Tonomura, J. Endo, T. Matsuda, T. Kawasaki & H. Ezawa in 1989.)

- It should be noted that if one slit is closed in a double slit experiment, the diffraction pattern disappears. So, when both slits are open, one may infer that the particle's wave had used "both" slits and created the diffraction pattern.




This is what people imply when they say the particle is not localized at one place, but has finite probability of being everywhere. Its more of particle not having a well defined single line trajectory, but made of waves of single or many wavelengths. As the size and distance between the slits are of the order of $\lambda/p$, we can probe these short-wavelength waves associated with the particle.

## Probabalistic / Superposition Interpretation

Let us return to the probabalistic interpretation of the above diffraction pattern of particles. As the particle approach the two slits and having the wavelength of the particle comparable to the distance between the two slits, the particle is now exposed to two possibilities, with equal or different probabilities, to pass through. In otherwords, the double slit instrument offers two distinct states to the particle, or the outgoing particle has two distinct states, and the total wavefunction is a linear superposition of the two distinct states $\varphi_1$ & $\varphi_2$ as

$$\psi(x) = c_1 \varphi_1(x) + c_2 \varphi_2(x) \qquad -(2)$$

where $c_1$ & $c_2$ are the coefficients or probability amplitude associated with two slits. We absorb $c_1$ & $c_2$ within $\varphi_1$ & $\varphi_2$.

Eq(2) can be interpretated as a linear "superposition" of two distinct possible states of the particle, implying that the particle have finite probability of being in any one of the state. If slit 2 is closed, then $c_2 = 0$ & $c_1 = 1$. and vice versa.

In this discription assinging a wavefunction with a

particle trajectory means, we are adopting a probabilistic approach. So, at what position particle will be detected on the screen can not be definitely ascertained, but we can only evaluate the probability of detecting at a position $P(x)$. By probability we mean the number of times that the particle will be detected at $x$ devided by the total number of measurements. The intensity of the pattern formed on the screen is proportional to $P(x)$.

From the theory of diffraction of light (wave), we know that the probability density $\propto$ intensity is given by

$$P(x) = |\psi(x)|^2$$

$$= |\phi_1(x) + \phi_2(x)|^2$$

(. ($c_1, c_2$ are absorbed in $\phi_1, \phi_2$))

$$= |\phi_1|^2 + |\phi_2|^2 + 2\,\mathrm{Re}(\phi_1^* \phi_2)$$

$$= P_1 + P_2 + (\text{Interference term})$$

Interference term:

Since $\phi_1$ & $\phi_2$ are complex functions, so we can write

$\phi_1 = |\phi_1| e^{i\theta_1} = \sqrt{P_1}\, e^{i\theta_1}$

$\phi_2 = |\phi_2| e^{i\theta_2} = \sqrt{P_2}\, e^{i\theta_2}$. Then we have

$$\boxed{P(x) = P_1 + P_2 + 2\sqrt{P_1 P_2}\cos(\theta_1 - \theta_2)}$$

The classical result would simply be $P_1 + P_2$, while the the quantum mechanics predicts a probability distribution oscillating between $|(\sqrt{P_1} - \sqrt{P_2})|^2$ to $|\sqrt{P_1} + \sqrt{P_2}|^2$ ie, between 0 to $4P_1$ if $P_1 = P_2$.

⊛ Now we, hypothetically, design an experiment that if the particle pass through Slit 1, it will obtain a color red, otherwise blue. Then in the detector we count them differently and plot the total probability. Then obviously we will measure $P = P_1 + P_2$ as we plotted in Fig 3 b. Mathematically, we say the total wave function $\Psi = c_1\Phi_1 + c_2\Phi_2$ has "collapsed" into any one of the state by distinguishing them. $c_1^2 + c_2^2 = 1$ This is to say by distinguishing them we are making $c_1$ or $c_2$ to be zero. We will see mathematical definition of collapsing a generic state into a given state.

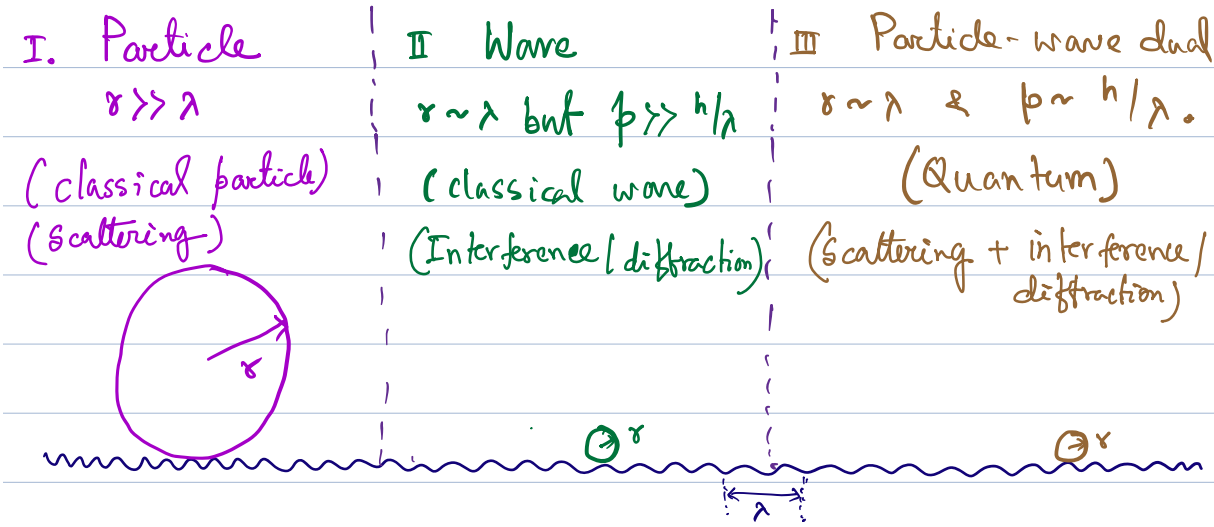
In modern language, the superposition of a state into two (or many) possible state can cause fractionalization of the particle. (Fractionalization of its charge, spin etc. The superposition of the two or many possible states also mean those two states hence generated remain entangled for ever, ie they know each other

no matter how far the screen is distanced from the slit. In another way to say, if we somehow find a way to measure one of the state, at very far away and after a long-long time later, we also certainly know the other state as well, since the total probability is 1.

- Double slit experiment and the wave nature, complex probability, superposition etc are the foundation of modern Quantum Mechanics. The "ad hoc" quantization rules of Bohr-Sommerfeld quantization, energy quantization, angular momentum quantization are part of the old quantum mechanics that we can reproduce by using modern QM.

[A close analog of a wavefunction of a "particle" is to consider a particle as some vector, say $\vec{A}$. Now, as the particle is exposed to two possible slits/states in the above example is to define the vector $\vec{A}$ in a 2-dimensional coordinate system with two linearly independent unit vectors $\hat{x}$ & $\hat{y}$ as $\vec{A} = A_x \hat{x} + A_y \hat{y}$. The analogy is $\vec{A} \equiv \psi$, $\hat{x}, \hat{y} \equiv \varphi_1, \varphi_2$ & $A_x, A_y \equiv c_1, c_2$. Collapsing a state $\psi$ into a given state is then equivalent to measuring $\vec{A}$ along a given axis. Indeed $\varphi_1, \varphi_2$ will be called vector space & $\psi$ as state vector]

# Summary & An Example:




Let us say we have a bumpy road, and a car is moving on it. We have three possible situations as shown above.

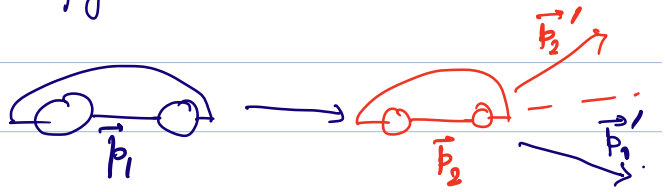
I. When the car's wheel size is much much bigger than the size of the bump, the car's vibration is negligibly small and thus although the vibration exists, but one does not feel / measure it. This is the classical limit of Newtonian mechanics, where the wave nature of the trajectory is not measurable due to the instrument's (wheel's) inability to resolve the small scale vibration. So, here the car moves as a particle and scatter with another car.

II. In the second situation, the wheel's size is now comparable to the bump's size. Here, the car will really vibrate wildly and all the passengers will be able to sense the vibrations. Therefore, the car's trajectory is defined by a wave solution. But we may not have yet reached the quantum limit unless the momentum is not low enough to reach the De Broglie limit of $p \sim h/\lambda$. $h \sim 10^{-34}$ J/sec. On regular road, the bump size is $\lambda \sim 1$ m. Then a car of 1 kg need to acquire speed $v \sim h/m\lambda \sim 10^{-34}$ m/sec to reach the quantum limit. Therefore, the wave nature of the car's trajectory is a classical wave. If many cars collide on such a bumpy road, the scattered cars will exhibit interference patterns - but this is still not a quantum limit where uncertainty principles will apply.

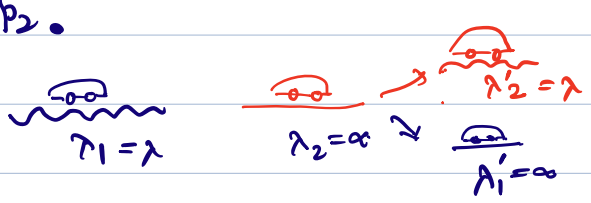
III. Let us now imagine an hypothetical situation where the bump's size and the car's size have been scaled to the atomic limit such that $\sigma \sim \lambda$ as well as $p \sim h/\lambda$. Then the car will acquire a particle and wave dual behavior. Now if the cars will exhibit both inference/diffraction as well as Compton & Raman scattering phenomena. Car's position and momenta will also not now be simultaneously determined with arbitrary precision.

**Compton Scattering:** Let us now try to perform a Compton like scattering between two cars on a bumpy road. We consider two situations.

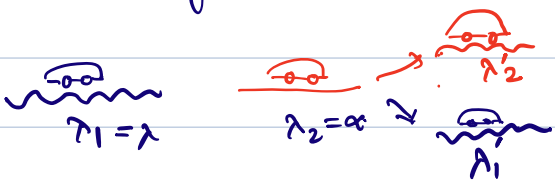
I. A classical car when it hits another car, they exchange momentum and both scatter with different momenta with the total momenta being conserved: $\vec{p}_1 + \vec{p}_2 = \vec{p}_1' + \vec{p}_2'$.



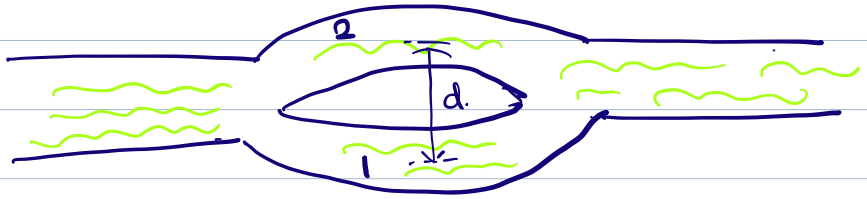

II. When a classical wavey car hits another car at rest, it exchanges its total wavelength and the second car vibrating at the same wavelength. Recall that this is what one expects in the Compton experiment to have only one peak at the same wavelength from classical wave theory.




III. But in the quantum limit, when two quantum cars hit each other they scatter like a particle, i.e. they exchange momenta and then both scatter into different wavelengths according to the momentum conservation, roughly, as $\frac{h}{\lambda_1} + \frac{h}{\lambda_2} = \frac{h}{\lambda_1'} + \frac{h}{\lambda_2'}$. This is what one observes in Compton effect.



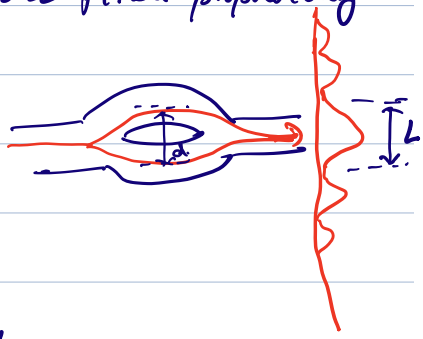
# Double Tunnel experiments with Cars:




Let us now imagine a bumpy road which splits into two (or have two tunnels on the road) before it's join again. How will the above three cars will travel after it cross the splitter ?.

I. The classical car will take either path 1 or path 2 and then move forward with a well defined trajectory. Despite the fact that the car had equal probability to choose between the two paths, but the final result does not depend on which path a car takes. If we observe many many cars, we will find that on average half of the cars will take path 1 & other half will take path 2, but all the cars will eventually meet at the same road and the total probability of finding all cars on the road after the splitter will add to 1.

II & III : In both Case II & III, we have a wave nature of the car's trajectory. Therefore, a car takes both the paths and the two split waves then merge to form diffraction pattern in the final path. Therefore, the car has a finite probability of finding it outside the path. The width of the spread L in the probability distribution is inversely proportional to d. Clearly, to see the diffraction pattern the distance d has to be of the order of the wavelength of the car. It is worthwhile repeating that the diffraction pattern is formed by a each car, due to its wave nature and simultaneously taking both path 1 & path 2. However, the intensity of the diffraction pattern will be too low to observe, and one needs enough number of car's diffraction process to observe appreciable intensity of the diffraction pattern.




( I am not sure if there is a way to distinguish between a classical wave and a quantum wave via double slit experiment)