Modern Physics: Part II: Atomic Structure

This world comprises of matter and energy; matter is defined with its smallest constituents called Atom which is electrically neutral and exhibits uniform chemical property. The concept of atom is ancient and was evolved philosophically. In 1804 John Dalton explained chemical reactions involving elements in ratios of whole number with the concept of atom. In 1897 when J J Thomson discovered electrons, understanding of atoms took a new turn and this continued with a series of independent hypotheses and experimental discoveries. These discoveries form another set of revolutionary thought experiments, in the form of fantasy based on scientific analysis and understanding of known practical observations. Later, the study of atom took two different directions. One of the directions is into physics which involves organization of elementary particles in atoms alongwith charges, forces and energies associated with them. The other direction is into chemistry which focuses on the impact of structure of atoms into their chemical affinity causing composition and decomposition into molecules. Both of them are complementary to each other.

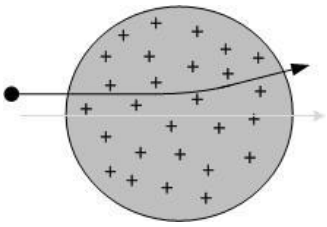
In this manual, upto this point, generally it has been possible to relate how? and why? of illustrations of subject matter using concepts covered in previous chapters of this manual. But, modern physics is a very complex matrix to be handled sequentially in a similar manner. Nevertheless, it is our endeavor to continue with the convention in this section too. However, resolving conceptual notches in content and scope wherever found to be making the trajectory too far, they have been supplemented in Appendix on Quantum Mechanics, an integral part of this section. Desperate readers, needing more details are requested to please come up with their inquisitiveness through CONTACT US. We are committed to pacify them suitably.

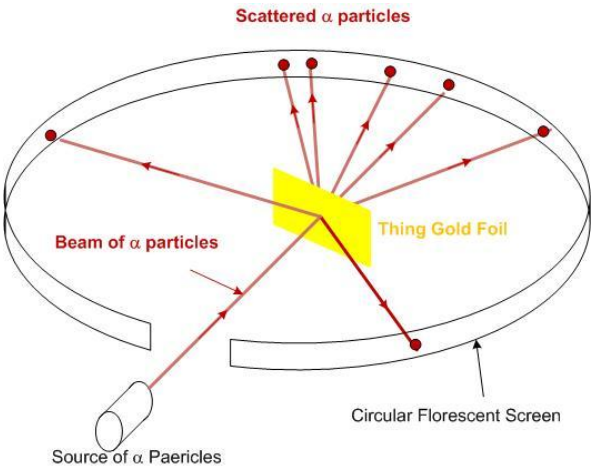
Introduction: Departure in understanding of physics, from classical approach, started in late Nineteenth Century and it took shape with Six revolutionary hypotheses – Quantization of radiation by Max Planck in 1900, Special Theory of Relativity with Photo Electric Effect by Albert Einstein in 1905, Louis de Broglie in 1924 with duality of particle and wave, Weiner Heisenberg on 1927 with Principle of Uncertainty and Erwin Schrödinger with wave equation in 1926. There were a galaxy of scientists who made invaluable contributions through experimental verification of these hypotheses to unfold arrogance of ignorance and thus creating new horizons for imagination. Accordingly, journey into the subject shall start with ***Structure of Atom***, with an appendix on **Quantum Mechanics**. It would leave much more to imagine and explore as one move forward in the journey.

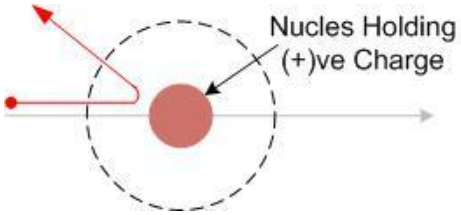
Structure of Atom: Matter is composed of tiny particles अणु परमाणु, in era of science being called molecule and atom, is available in ancient scriptures. A scientific understanding started with study of behavior of gases by **Robert Boyle** in 17th century where he explained compressibility of gases with its tiny particles filling available volume with lot of spacing between them. **John Dalton** in 1800 proposed concept of atom to explain why element in fixed proportion whole number participate in reactions. It was in 1827, **Robert Brown** microscopically studied erratic motion of dust particles in water, in 1827, known as **Brownian Motion** forming basis of *Kinetic Theory of Gases*. Beyond this, *the Brown's theory validated the Dalton's proposition of atom*.

In 1898, **J.J. Thomson**, while conducting experiments with cathode rays proposed structure of atom as a solid sphere carrying (+)ve charge with electron holding (-)ve charge embedded in it to exhibit electrically neutral charge. This model could explain emission of electrons as well as ionization and formation of chemical

compounds. **Philipp Lenard** in 1903 while experimenting effect of cathode rays directed towards a thin film. He observed that some of electrons were passing through the film and thus proposed empty space in atoms allowing passage to the electrons. **Ernest Rutherford**, while bombarding **α-particles,** nucleus of Helium atoms, on gold foil, observed that most of alpha particles either passed through the foil or with small deviation as shown on the figure. Then an understanding of α-particles was incomplete except that they are naturally emitted by radioactive material, and that they carry (+) charge and are ejected by unstable atoms at a speed of about 10^7 m/sec. These particles could travel several cm in air and upto 0.1 mm thin solid material. ***Protons and Neutrons***, a constituent **α-particles** was discovered later in 1918 and 1930, respectively. Probability of straight reflection of **α-particles** was about 1 in 1800. And, in 1911, Rutherford estimated that the **α-particles** is about 7350 times heavier than electron. Thus neither the electron nor (+)ve charged particles could cause large scale deflection. But, the direct rebounding at an angle of deflection 180^0 was indicative of head-on collision with much heavier mass carrying (+) charge which occupy small space at the center of atoms of the material of the foil. Further, he estimated that the size of this central mass, and was later called as **Nucleus** of size 10 Fermi (1 Fermi=1 Fermi = 10^{-15}m) and about 10^{-5} of the size of the atom, and thus empty space in atom around its nucleus was about 10^{-15} times of its size, by simple cubic proportion as per geometry.

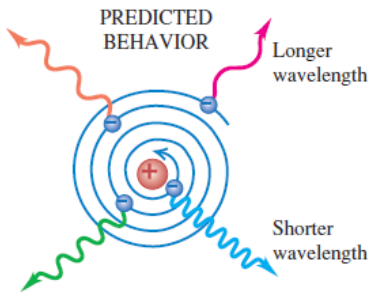






This formed the basis of Nuclear Model of atom, according to which: atom comprises of a concentrated mass called Nucleus having (+)ve charge. Remaining volume of the atom outside nucleus is occupied with electrons at a separation revolving around the nucleus. Number of electrons is such that it equalizes charge on nucleus so as to maintain each atom to be electrically neutral. This provides an explanation of easy emission of electron. Moreover, electron revolving around nucleus in circular orbit provides stability of the atomic structure, caused by equilibrium of electrostatic (centripetal) forces and centrifugal force caused by circular motion.

Limitations of Rutherford's Model: These experimental observations of Rutherford contradicted Thomson's model of distributed mass within the volume of atom. But, this model again did not survive the logical argument: **a)** What prevents electron to fall into positively charged nucleus, under the action of persistent electrostatic force of attraction*;* **b)** If electron are revolving around nucleus, it is possible only on account of persistent centripetal acceleration, and an accelerated charged particle must emit radiation in accordance with theory of electromagnetic field. *But, no such radiation coming out of stable atoms is observed;* **c)** This radiation of energy should lead to loss of kinetic energy of revolving electrons and eventually decrease in radius of the orbit of revolution till it collapses into nucleus. *This does not happen and the atom continues to be stable;* **d)** Reduction in radius of orbit should produce a continuous

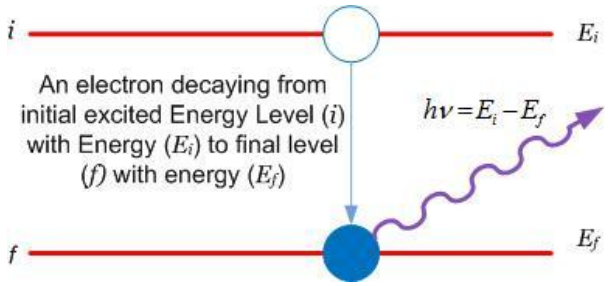


spectrum of radiation and reduction in volume of atom, with the passage of time, creating high density material, *which does not happen*.

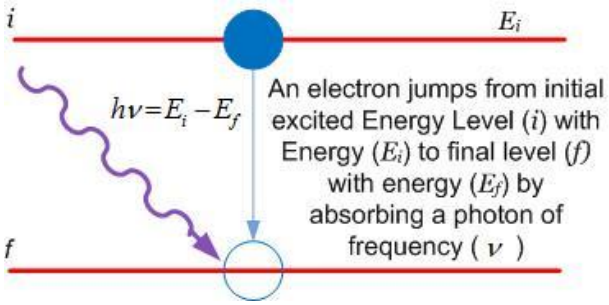
Spectral Lines: A heated metal radiating a continuous spectrum, is an observation since immemorial times. Experimenting with heating of hydrogen in sealed tube, **Johann Balmer**, in 1885 observed discrete emission spectral line, each corresponding to a particular wavelength, known as **Balmer Series**. Later in 1906, **Theodore Lyman** observed another set of spectral lines. Soonafter, in 1908, **Friedrich Paschen**, discovered another set of spectral lines. Wavelengths were fitted into an empirical formula $\frac{1}{\lambda} = R\left(\frac{1}{n^2} - \frac{1}{m^2}\right)\ m^{-1}$, where, $R = 1.0973 \times 10^7\ m^{-1}$ is known as Rydberg's constant. In similar experiments in **Sumner Brackett** and **August Herman Pfund** discovered new set of spectral lines in 1922 1nd 1924, respectively. Until Bohr could make a sense of these spectral lines to propose structure of atom, discussed below, they remained mystery and a subject of experimental curiosity. Accordingly, elaboration of these spectral lines is deferred until Boh'r is discussed.

Spectral Lines	m	n
Balmer Series	2	1
Lyman Series	>2	2
Paschan Series	>3	3

Boh'r Model: Neil Bohr, who was working with Rutherford, advanced a hypothesis, in 1913, which made a sharp turn from pure classical mechanics with the amalgamation of quantum mechanics into it. The hypothesis was based on a premise that – "*energy of an atom can have only discrete values*". This hypothesis had bearing on spectral lines discovered upto Lyman Series. Accordingly he suggested that :

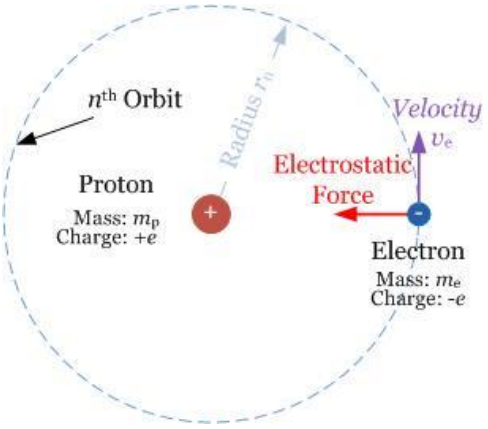


- **a.** Sharp observation of spectral lines on hydrogen is attributed to photon of energy $\boldsymbol{E = h\nu}$ emitted/absorbed by hydrogen atom.
- **b.** During emission of a photon internal energy of an atom is reduced by a quantum equivalent to E.
- **c.** Each atom must be able to exist in states of specific values of internal energy.
- **d.** There are a set of possible energy levels and internal energy of atoms corresponding to each of the discrete energy level occupied by electrons in an isolated atom. No electron can stay in any position which is intermediate to discrete Two energy levels.
- **e.** All isolated atoms of any element have some set of energy levels, but different elements have different set of energy levels.
- **f.** An atom can be excited from one energy level (E_i) to another level (E_f) by imparting energy through by heating, collision of an atom by an accelerated particle. This excited atom makes transition to lower discrete energy level by emitting a photon of wavelength corresponding to difference of energy between two energy levels such that $\boldsymbol{h\nu = E_i - E_f}$.

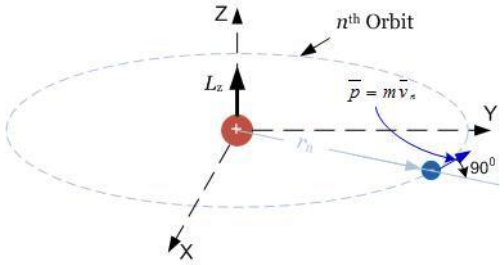


Bohr hypothesis while relating atomic spectra to energy levels of Hydrogen, the simplest atom, he combined quantum mechanics with classical electromechanics. The force of attraction between electron revolving, around nucleus having a proton, in n^{th} orbit of radius r_n in accordance with *Coulomb's Law* is $F = \frac{1}{4\pi\epsilon_0} \cdot \frac{e^2}{r_n^2}$ N, and acts as

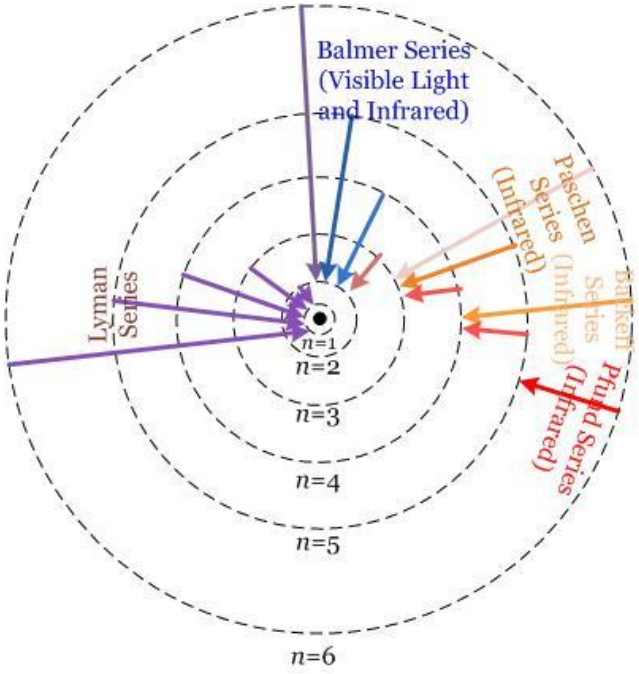
centripetal force. While performing circular motion the electron experiences a constant acceleration $\frac{v_n^2}{r}$ radially directed towards center of the orbit. Accordingly, as per Newton's Second Law of motion, a centrifugal force comes into play which creates equilibrium for electron to continue to perform circular motion. Thus equation of equilibrium of electron having mass m, is $\frac{1}{4\pi\epsilon_0}\cdot\frac{e^2}{r_n^2}=\frac{mv_n^2}{r_n}\rightarrow r_n=\frac{4\pi\epsilon_0 m}{e^2}\cdot(v_n r_n)^2$.



As per quantum mechanics, Bohr quantized angular momentum of electron as $L_n=mv_n r_n=n\frac{h}{2\pi}\rightarrow v_n r_n=n\frac{h}{2\pi m}$. Combining this with the equation of force, $r_n=\frac{4\pi\epsilon_0 m}{e^2}\cdot\left(n\frac{h}{2\pi m}\right)^2=\epsilon_0\frac{n^2h^2}{\pi me^2}$, is the radius of the n^{th} orbit such that $r_n\propto n^2$ and velocity on electron in the orbit would be $v_n=\frac{1}{\epsilon_0}\cdot\frac{e^2}{2nh}$. Radius of 1st orbit is called Bohr's radius $a_0=5.29\times10^{-11}m$, using predefined values of $\epsilon_0=8.854\times10^{-12}\mathrm{C^2N.m^2}$, $h=6.624\times10^{-34}\mathrm{J.s}$, $m=9.109\times10^{-31}\mathrm{Kg}$, and $e=1.6028.854\times10^{-12}C^2\mathrm{N.m^2}$ Thus permitted radii for orbiting electron are $r_1=a_0$, $r_2=4a_0$, $r_3=9a_0$, and so on.

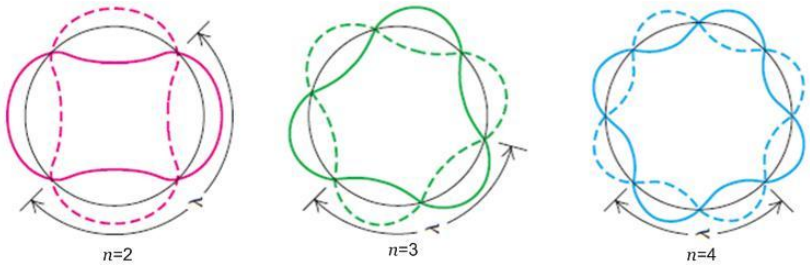


Now, extending *Bohr's Model* to the analysis of energy (E_n) of an electron at n^{th} energy level. It has Two components, Potential Energy $E_{Pn}=-\frac{1}{4\pi\varepsilon_0}\cdot\frac{e^2}{r_n}=-\frac{1}{\epsilon_0^2}\cdot\frac{me^4}{4n^2h^2}$ and Kinetic Energy $E_{Kn}=\frac{1}{2}mv^2=\frac{1}{\epsilon_0^2}\cdot\frac{me^4}{8n^2h^2}$. Thus total energy of the electron $E_n=E_{Pn}+E_{Kn}=-\frac{1}{\epsilon_0^2}\cdot\frac{me^4}{8n^2h^2}=-\frac{hcR}{n^2}$, here, $R=\frac{me^4}{8\epsilon_0^2}$ is an analytically determined constant is conforming to empirically determined Rydberg's constant. Accordingly, as postulated by Bohr, $h\nu=\frac{hc}{\lambda}=E_n-E_m=hcR\left(\frac{1}{n^2}-\frac{1}{m^2}\right)\rightarrow\frac{1}{\lambda}=R\left(\frac{1}{n^2}-\frac{1}{m^2}\right)$, here λ is the wavelength of radiation emitted by an electron decaying from mth orbit to nth orbit. This striking coincidence in empirical constant and analytically determined constant is amazing. Accordingly, sets of spectral lines in isolated hydrogen atoms emitted by electron decaying from higher energy level through intermediate levels to ground level are shown in the figure below. Similar spectral lines were observed in hydrogen like atom having one electron in outermost orbit.



Quantization of angular momentum by Bohr as an integral multiple of $\frac{h}{2\pi}$, which makes a way to wave nature of electron predicted by Broglie, discussed in Appendix, according to which electrons instead of moving strictly in circular orbit perform sinusoidal motion as a standing wave having integral wavelengths such that $2\pi r_n=n\lambda_n$.

Thus, revisiting the angular momentum leads to wavelength of an electron in n^{th} orbit as $mv_n r_n = n\frac{h}{2\pi} \rightarrow 2\pi r_n = \frac{nh}{mv_n} = n\lambda_n \rightarrow \lambda_n = \frac{h}{mv_n}$. Wave nature of electrons in orbit is shown in the figure. Together with this *Heisenberg's Uncertainty,* elaborated at Appendix, and *Schrödinger Wave Equation, introduced at Appendix,* detailed description of atomic structure runs outside the scope of this manual. Bohr's model though good enough to explain hydrogen atom is insufficient to explain structure of atoms having more than one electron.



Limitation of Bohr's Model: Bohr's model together with wavelength of spectral lines provided by the model is reasonably accurate and is a good justification for preliminary acceptance of Bohr's model even today. But, it suffers from following limitation for a universal acceptance :

- **a.** It fails to explain why does orbiting electron experiencing constant centripetal acceleration does not decay into nucleus.
- **b.** Wavelengths of spectral lines for hydrogen are very close to actual as shown earlier. But, prediction of spectral lines for larger atoms is very poor,
- **c.** It assumes orbital position of electron, its velocity and momentum to be certain, which is impossible as per *Heisenberg's Uncertainty Principle*.
- **d.** It fails to predict Zeeman Effect and Stark Effect causing splitting of spectral lines in presence of magnetic field and electric field, respectively. Both these effects are excluded in present elaborations, being outside the domain of this manual.

Illustration of ***Zeeman Effect*** and ***Stark Effect*** together with the reason as to why stable atoms do not emit radiation is beyond the scope of this manual. Nevertheless, quarries of inquisitive readers are invited through *CONTACT US.*

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APPENDIX – Quantum Mechanics

Aim of this Appendix is to make concepts of Quantum Mechanics contextual for elaboration of modern physics. While evolving this appendix care has been taken to limit the discussions within the scope and concepts covered in this manual. It is requested that this may not be treated as complete text of the concepts, which are much beyond.

In 1900, hypothesis of **Max Karl Ernst Ludwig Planck,** also referred as ***Max Planck*** and ***Karl Planck***, in which he quantized radiation of energy, be it emission or absorption, is in the form packets calling them **Quantum**. This concept with contribution of many scientists developed into **Quantum Mechanics**, a branch of Physics. Prior to Planck, in 1887, **Heinrich Hertz** experimentally demonstrated emission of electrons from metal surface on incidence of light, and it was christened as **Photo Electric Effect**. *This would be dealt with separately in the next chapter*, nevertheless it is essential to make its relevance into motivation to Planck to propound his hypothesis of Quantum of Radiation.

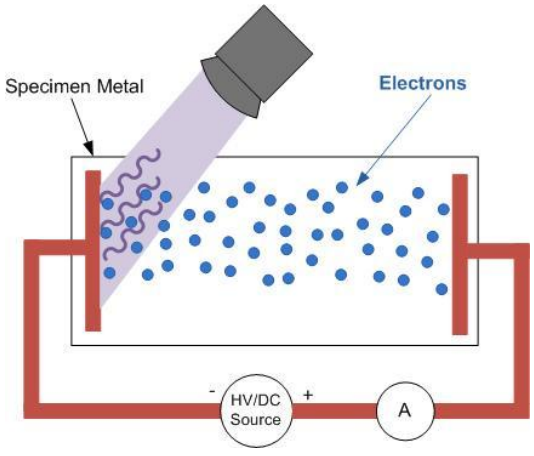
It was observed by Hertz that when light falls on a metal surface, under certain conditions, there is emission of electrons. It had following characteristics –**a)** Photo electric effect occurs only on incidence of light above a fixed frequency, called *Threshold Frequency (v_0),* and not below that; **b)** The emission of electrons is **instantaneous** on incidence of light; **c)** Minimum Kinetic Energy is independent of intensity of light. These observations contradict inferences of classical mechanics and also Maxwell's Electromagnetic Field Theory which propounds that – **a)** Transition from of state occurs on gain or loss of sufficient energy, called *Threshold Energy* (∅), either in impulse or a gradual and incremental process, **b)** The gradual process shall take some time to attain the threshold energy and cannot be instantaneous, **c)** Decrease in intensity of light with increased time of incidence will not cause accumulation of light energy to initiate emission of electron. Elaboration of Photo-Electric Effect here is contextual to build premise of Quantum Mechanics, crucial in understanding of atomic structure. Nevertheless, details of this effect shall be dealt with in next chapter.

These contradictions were motivation to ***Planck*** to advance hypothesis of Quantization of Electromagnetic Radiation and light is part of its spectrum, while he was studying **black body radiation**. He stated that "A black body radiation chamber can be supposed to be filled up with harmonic oscillators each with a characteristic frequency (known as Planck's Oscillators). Energy of each oscillator cannot change continuously but is limited to a discrete set of values which are integral multiple of small unit of energy called quantum of radiation. Accordingly, plank proposed a constant ***h*** known as Planck's Constant.

In 1897, J.J. Thomson during his experimented with cathode rays under combined influenced of magnetic and electric field, using Coulomb's Law and Ampere's Force Law. He discovered negatively charged particles calling them corpuscles having a mass 1840 times a Hydrogen atom, then available knowledge of electro-magnetic interaction. At that time, presence of subatomic particles was not accepted. Further, he determined ratio of charge to mass of these corpuscles $\frac{e}{m} = 1.7588196 \times 10^{11}\ \mathrm{C.kg^{-1}}$. It was only in 1909 when Robert Millikan measured charge of an electron and currently accepted value **e= -**1.6021773×10^{-19} C through a famous Oil Drop Experiment. This helped to accurately determine value of $h = 6.626096896(33) \times 10^{-34}\,\mathrm{J.s}$.

Understanding of interference, diffraction and polarization is well substantiated by wave theory. But, inability of the wave theory to explain scattering effect and contradictions surfaced in Photo-Electric Effect, and associated experimental observations were a beginning attributed to Planck, with a distinguished hounour of being called ***Father of Quantum Mechanics***.

Discovery of Photon: Photo-Electric Effect is being briefly visited to take forward the concepts of quantum mechanics. An evacuated tube with two separated electrode when electric potential difference is applied across them no current is established. But, as soon as the electrode at (-)ve potential is illuminated, small current established across the electrodes. Stopping of this current, requires a minimum reverse voltage called **stopping voltage** ($\boldsymbol{V_0}$), such that $\frac{1}{2}m_e v_{max}^2 - eV_0 = 0$, or $v_{max} = \sqrt{\frac{2eV_0}{m_e}}$. Here, $\boldsymbol{m_e}$ is mass of electron, $\boldsymbol{e}$ is charge of electrons and v_{max} is the maximum velocity attained by electron by incidence of light.

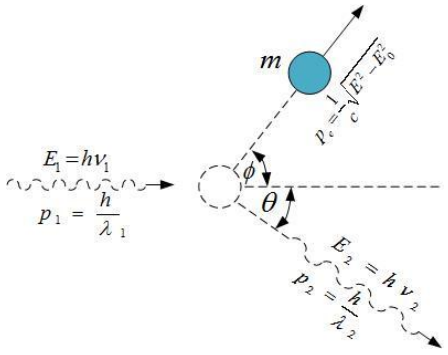


Albert Einstein in 1905 used Planck's hypothesis to explain photo electric effect and suggested that every cycle of an electromagnetic

radiation is an energy packet with energy content $E = h\nu$; here E is the energy of the packet, and this equation is ***Planck-Einstein Relation***. This energy packet was termed as ***Photon***, after about Two decades on 1926 by **Frithiof Wolfers** and **Gilbert N. Lewis** . Ever since Arthur H Crompton was awarded Nobel prize on 1927, for his studies on scattering of light independent existence of photon, a packet of electromagnetic energy. According to Einstein's theory individual photon is either fully absorbed by a single electron or nothing; there is neither accumulation nor sharing as per wave theory. An electron to escape requires minimum energy called Work Function ($\emptyset$) and is different for each metal, Later in this chapter difference of $\emptyset$ across different metals shall be seen to be on account of their atomic structure. Thus energy balance equation $h\nu = \emptyset + \frac{1}{2}m_e v^2$ represents effect of an incident photon. This provides answer to minimum stopping potential as $V_0 = \frac{\frac{1}{2}m_e v_{max}^2}{e} = \frac{h\nu - \emptyset}{e}$. In this equation driving factor for photo-electric effect is frequency of radiation and not its intensity. This concept of photon is applicable over complete spectrum of electro-magnetic radiation. As per special theory of relativity, a particle with Zero Rest Mass has eventually velocity $\boldsymbol{c}$, its momentum-energy correlation is $E = pc$, where E and p are energy and momentum of photon. Since, $E = h\nu$ it leads to $h\nu = pc \rightarrow h\frac{c}{\lambda} = pc \rightarrow p = \frac{h}{\lambda}$. Here, momentum ($p$) being a vector has same direction as that of its velocity. *This concept shall go a long way into understanding of atomic structure.*

Understanding of Photon Effect created an obvious intuitive corollary among the contemporary scientists, as to can energy imparted metal cause emission of Photon. **Wilhelm Röntgen**, while experimenting with Cathode Rays observed in 1895, observed that a cathode when provided with thermal energy equal to its work function ($\emptyset$), a thermionic emission of electrons takes place. These electrons, under vacuum and under high potential difference, bombard on anode with high velocity and a radiation is produced in support of the corollary. Since, characteristics of this radiation was not known, it was called X-Rays. In this appendix efforts is to build context of Quantum Mechanics, more elaboration of X-rays would follow in the next section.

Particle Nature of Photon: In 1922 **Arthur H Crompton** in an experiment aimed X-rays beam at a solid target recoded lower frequency radiation at points with angular displacement with the path of X-ray. This was in contradiction to wave theory which propounds absorption of radiation by an electron sets it in oscillation in response to electric field of EM radiation. The oscillating electron in turn radiates energy in all directions, like an antenna, in the form of EM waves of same frequency. Crompton observed that for an incident radiation of wavelength $\boldsymbol{\lambda}$ the scattered radiation at an angle $\emptyset$ with the line of incidence having wavelength $\boldsymbol{\lambda'}$ satisfied a relation: $\lambda - \lambda' = \frac{h}{mc}(1 - \cos\emptyset)$. This equation is mathematically sustainable using principles of elastic collision and relativistic mechanics. Taking $\bar{\boldsymbol{p}}$ and $\bar{\boldsymbol{p}}'$as momentum vectors of incident and scattered photons having magnitudes $\boldsymbol{p}$ and $\boldsymbol{p}'$, respectively. Electron, which was initially at rest with rest mass $\boldsymbol{m}$, is like a packet of energy $\boldsymbol{E_0 = mc^2}$. After impinging of photon the electron gains a momentum vector $\overline{p_e}$ having magnitude $\boldsymbol{p_e}$ and an energy $= \boldsymbol{p_e c}$, as per relativistic principles. As per conservation of momentum. $\bar{p} = \bar{\bar{p}}' + \overline{p_e}$. This as per vector algebra $\overline{p_e} = \bar{p} - \bar{\bar{p}}'$ and $p_e = \sqrt{p^2 + P'^2 - 2p \cdot p_e \cdot \cos\emptyset}$. As per conservation of energy, total energy of photon-electron system is $pc + mc^2 = p'c + E_c$. Here, the energy of electron post collision is: $E_c = \sqrt{(E_0)^2 + (p_e c)^2}$, in accordance with



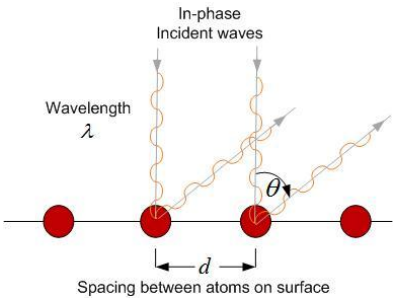
relativistic energy-momentum relation. It leads to $E_c^2 = (E_0)^2 + (p_e c)^2 \rightarrow (mc^2)^2 + (p_e c)^2 = (pc + mc^2 - p'c)^2$. Substituting value of p, above in this equation and squaring it square of terms pc, $p'c$ and mc^2 would cancel out, leaving behind: $pmc^3 - p'mc^3 = pp'c^2 - pp'c^2 \cos\emptyset$. Dividing this equation in reduced form with $pp'c^2$, final form of this equation is $\frac{mc}{p} - \frac{mc}{p} = 1 - \cos\emptyset$. Further, multiplying by $\frac{h}{mc}$ to this final form $\frac{h}{p} - \frac{h}{p'} = \frac{h}{mc}(1 - \cos\emptyset)$. Using the relativistic definition of wavelengths the equation becomes $\lambda - \lambda' = \frac{h}{mc}(1 - \cos\emptyset)$, and this is same as concluded by Crompton.

Thus Crompton combined Einstein' Theory with classical mechanics. *This turned out to be first step to propound* ***dual nature of Photon*** *i.e. a particle as well as a wave.*

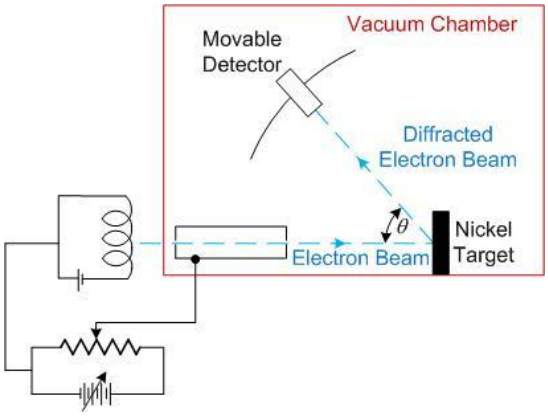
In 1933, **Patrick Blackett** and **Giuseppe Occhialini** observed that when Gamma radiation, which constitutes highest frequency of radiation, when is incident on a target, it may not scatter, instead it may disappear completely and a new pair particles are created an electron and a positron both having equal mass but with opposite charges. Thus the pair maintains electrical neutrality of the process. Thus, minimum frequency of radiation required to produce the pair conforms to equation: $E_{min} = h\nu_{min} = 2\left(\frac{1}{2}m_e c^2\right)$. This process is reversible, as much as collision of electron and proton causes decay of the two particles with emergence of a photon gamma radiation. Though, this phenomenon is unexplained in photo-electric effect, it is in conformance with center of momentum, where total momentum remains Zero.

Particle Behaving as a Wave: A natural consequence of above discoveries another obvious question was: can a particle behave like a wave? How an atom does remain stable despite ever accelerating electrons, due to centripetal force caused by their orbital motion? Does it not radiate energy like an accelerating charged particle?

In 1924, **Prince Louis de Broglie** (last name pronounced as **Broy**) made an hypothesis that: nature loves symmetry. Accordingly, light has a dualistic nature whereby in some situation light behaves like wave and in other like particle. It is in accordance with symmetry of nature of particle as wave, which is bound to have velocity, wavelength and frequency, essential parameters of a wave. Broglie postulated that a particle with rest mass $\boldsymbol{m}$ moving with a velocity $\boldsymbol{v}$ has a momentum has a momentum $p = \boldsymbol{mv}$. As per stipulations of quantum mechanics the particle should exhibit a wavelength $\lambda = \frac{h}{p} = \frac{h}{mv}$ and this is called **Broglie's Wavelength.** In the event of the particle attaining a velocity comparable to velocity of light (**c**), relativistic mass of the particle would come into play and thus momentum would be $p = \frac{m}{\sqrt{1-\frac{v^2}{c^2}}}v = \chi mv$, here $\chi = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$, is the Lorentz factor. Further, relativistic principle stipulates that $E = h\nu$, here, ν is the frequency, Thus, Broglie related momentum and frequency to the energy of the particle in the same way as that of the photon.



Three years later in 1927 **C.J. Davisson and L.H. Germer** during their studies with electron beam directed on a piece of metal observed strong maxima and minima at specific angles in conformity with diffraction pattern realized with a EM beam passed through a grating.

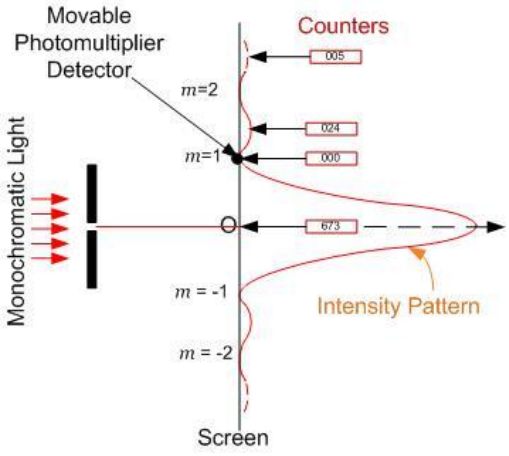


The speed of electron was determined from accelerating voltage $\boldsymbol{V_{ba}}$ using principles of classical mechanics and electro-statistics, kinetic energy of the electron is $\boldsymbol{KE = eV_{ba} = \frac{1}{2}m_e v_e^2 = \frac{p_e^2}{2m_e}}$. Here, $\boldsymbol{e}$ is the charge of electron. Accordingly, $\boldsymbol{p_e = \sqrt{2m_e eV_{ba}}}$. Thus, in accordance with Broglie's Wavelength, wavelength of the accelerated electron shall be $\boldsymbol{\lambda_e = \frac{h}{\sqrt{2m_e eV_{ba}}}}$. This clearly indicates that with the increase in accelerating voltage ($\boldsymbol{V_{ba}}$) wavelength exhibited shorter wavelength on electron wave, and is in conformity with the diffraction pattern. It in turn revealed that atoms near surface were arranged in row with a distance ($\boldsymbol{d}$)between them. Accordingly, occurrence of strong reflections $\boldsymbol{d \sin\theta = m\lambda}$ (m-1,2,3…) are identical to those with gratings with center-to-center spacing as $\boldsymbol{d}$**.** This diffraction pattern was the first evidence of Broglie's Hypothesis to be regarded as **Broglie's Principle**. In 1928, **G.P. Thomson** carried out different experiment on electron diffraction using polycrystalline metallic foil. While the electron beam passed through the foil it depicted a circular diffraction pattern around the beam reconfirming the Broglie's Hypothesis.

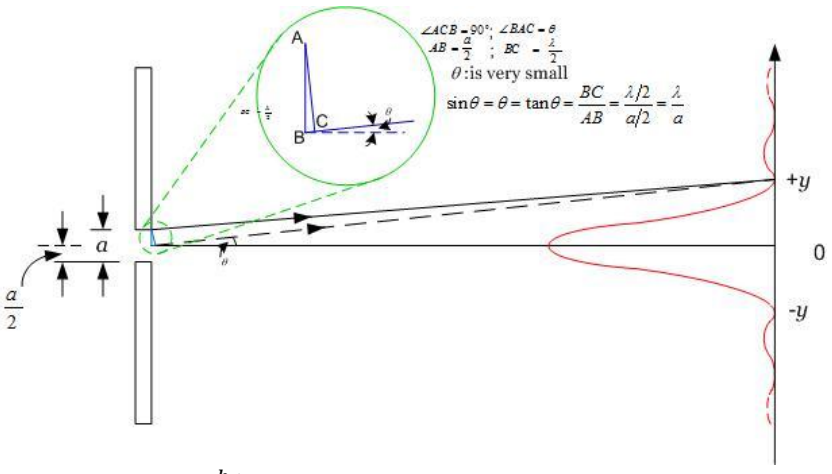
Electron Microscope: Using Broglie's Principle first electron microscope was invented, by **Max Knoll** and **Ernst Ruska** in 1931, to resolve objects smaller than possible with perfectly designed optical microscope, using wavelength of 500 nm. Since then there have been many developments in design to improve the resolution. An accelerated electron beam can reach wavelength many thousand times shorter than the optical limit. Thus electron microscope renders many thousand times larger magnification than that available with optical microscope. It is important to note that trajectory of electron can be determined based on classical principles of physics involving charged particles governed by electric and magnetic forces. It is only when resolution is the concern wave properties of electron are involved.

Wave Particle Duality, Probability and Uncertainty: The foregoing discussions open a new curiosity as to how can EM radiation can behave as a particle and a wave too. **Neils Bohr** in 1928 advanced a **Principle of Complementarity** which stipulates that: *in EM radiation both particle and wave models exist such that in any phenomenon of the radiation either of the Two model is operative, and both of them in concurrence*. This was demonstrated with single-slit diffraction pattern placing photon counters or alternatively photographic plate in place of screen used by **Fraunhoffer**; the wave model elaborated in section on Optics. It was seen that pattern of distribution of photons correspond to the intensity of light. Similar observation was obtained with double slit interference pattern in conformity wave model justifying the complementarity of the Two models.

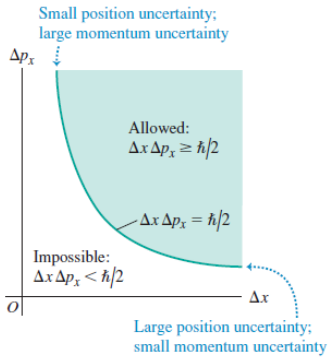
In classical mechanics an object is treated as a point mass which has energy and momentum, which makes it possible to describe motion of the particle at any time in space (X,Y and Z coordinates). But, Photon being considered to have a Zero rest mass, it cannot be treated as a point mass. This introduced uncertainty into path of photons having same initial state. This uncertainty is demonstrated both in position and momentum of photon and, therefore, an inseparable probability to the Two variables. In the single slit diffraction of a wave with wavelength $\boldsymbol{\lambda}$ through a slit of width a, first minima occurs at an angle θ_1 with the central line. At a sufficiently long distance from a narrow slit, it is seen that $\sin\theta_1 = \theta_1 = \frac{\lambda/2}{a/2} = \frac{\lambda}{a}$. Looking at this phenomenon, a photon striking at edge of first fringe, probability to its momentum along X-axis and Y-axis are assigned as p_x and p_y. Probability of a photon striking at edge of first fringe and central



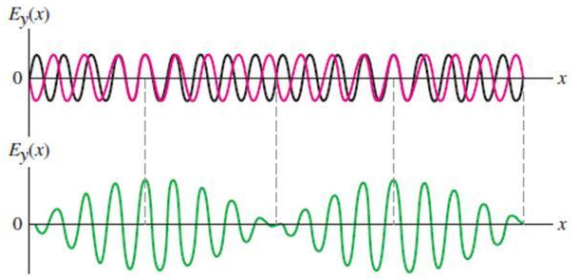
maxima and accordingly, $\tan\theta_1 = \theta_1 = \frac{p_y}{p_x} \rightarrow \frac{\lambda}{a} = \frac{p_y}{p_x}$. Photons striking detector within First minima around central maxima are within angle $(+)\frac{\lambda}{a}$ to $(-)\frac{\lambda}{a}$ are 85 %,such that all photons leaving the slit reach detector either above or below the central maxima and therefore $p_y\big|_{average} = 0$. Accordingly, uncertainty of a photon striking away from central maxima is $:\Delta p_y = p_x\frac{\lambda}{a}$. Relation between momentum of a photon and its wavelength is $\lambda = \frac{h}{p}$. Therefore, along the central line $\Delta p_y = p_x\frac{h/p_x}{a} = \frac{h}{a}$. This leads to an evident inference is narrower the slit larger is the probability of a photon striking away from central maxima; accordingly, a wider diffraction pattern.



Uncertainty Principle: In statistics uncertainty of a quantity is defined in terms of standard deviation. In 1927, **Weiner Heisenberg** postulated uncertainty in momentum and position of a photon to be $\Delta x\Delta p \geq \frac{\hbar}{2}$. Here, $\hbar$ (pronounced "h-bar") *is called* **reduced Planck constant** or **Dirac constant such that** $\hbar = \frac{h}{2\pi}$. It was another milestone in Quantum Mechanics which states that position and momentum of a particle are complementary and it is impossible to either with certainty. This is valid with any equipment howsoever sophisticated it may be. This was explained with a simple argument that any detector to be able to function has to interact with the particle. In the process there is moderation in state of the particle, and thus uncertainty becomes fundamental and intrinsic. This uncertainty is just not to be treated specific to X-axis, it is also valid in space and hence $\Delta y\Delta p \geq \frac{\hbar}{2}$ and $\Delta z\Delta p \geq \frac{\hbar}{2}$, as shown in the figure.



Wave Uncertainty: Equation of an EM wave propagating along X-axis with its electric field polarized along Y-axis as a function of position and time given by Maxwell is $E_y(x,t) = A\sin(kx - \omega t)$, already elaborated in Chapter on Waves and Motions. Here, $k = \frac{2\pi}{\lambda}$ and $\omega = 2\pi\nu$. In quantum mechanics frequency is invariable represented with symbol ν instead of f, unit being the same Cycles-per-second. These two parameters k can be expressed in terms of momentum of photon it leads to $p_x = \frac{h}{\lambda} = \frac{h}{2\pi}\cdot\frac{2\pi}{\lambda} = \hbar\cdot k$. Likewise, another parameter ω can be expressed as energy of the photon, leading to $E = h\nu = \frac{h}{2\pi}\cdot 2\pi\nu = \hbar\omega$. Thus the wave equation gets transformed into $E_y(x,t) = A\sin\left(\frac{(p_x x - Et)}{\hbar}\right)$. If a definite value us assigned to p_x, it leads to Zero uncertainty, expressed mathematically as $\Delta p_x = 0$. This is where Uncertainty Principle comes into play and probability of position of a photon



$\Delta x = \infty$. This leads to loss of nature of a wave where amplitude is uniform throughout the length of propagation, a total loss of information.

In diffraction pattern it has been observed that there is a known probability of a photon being found in a certain position. This calls for rewriting wave equation as with Two waves with slightly different wavelengths which can cause beats as elaborated in chapter on Waves and Motion, as: $E_y(x,t) = A_1 \sin\left(\frac{(p_{x1}\cdot x - E_1 t)}{\hbar}\right) + A_2 \sin\left(\frac{(p_{x2}\cdot x - E_2 t)}{\hbar}\right)$. Thus, at certain time say $t = 0$, $E_y(x, t=0) = A_1 \sin\left(\frac{p_{x1}\cdot x}{\hbar}\right) + A_2 \sin\left(\frac{p_{x2}\cdot x}{\hbar}\right)$. When $A_1 = A_2$, the nature of beats can be expressed as: $E_y(x, t=0) = 2A \sin\left(\left(\frac{p_{x1}+p_{x2}}{2}\right)\cdot\frac{x}{\hbar}\right)\cdot\cos\left(\left(\frac{p_{x1}-p_{x2}}{2}\right)\cdot\frac{x}{\hbar}\right)$. It leads to the probability of a photon being found at a place is maximum where amplitude is maximum and can be ascertained only by assigning probability to p_{x1} and p_{x2} in conformance with the Heisenberg's Uncertainty Principle $\Delta p_x . \Delta p_x \geq \frac{\hbar}{2}$.

Energy Uncertainty: The wave equation at $x = 0$, becomes $E_y(x=0,t) = A_1 \sin\left(-\frac{E_1 t}{\hbar}\right) + A_2 \sin\left(\frac{E_2 t}{\hbar}\right)$. It implies that: $E_y(x=0,t) = -A_1 \sin\left(\frac{E_1 t}{\hbar}\right) + A_2 \sin\left(\frac{E_2 t}{\hbar}\right)$. Thus electric field at a point is combination of Two oscillating fields with $\omega_1 = \frac{E_1}{\hbar}$ and $\omega_2 = \frac{E_2}{\hbar}$, is synonymous to beats referred to above. This equation also equally attracts Uncertainty Principle where $\Delta E \Delta t \geq \frac{\hbar}{2}$. Most likely a photon can be found at a time when amplitude is largest; the price of localizing photon in time is uncertainty of energy of wave.

Schrödinger Wave Equation: Around the same time when Heisenberg advanced Uncertainty Principle, In 1926 Erwin Schrödinger published a wave equation considering wave-particle duality equation and probability of finding a particle at a certain position. The Schrödinger Wave Equation is a mathematical model of quantum mechanical behaiour of sub-atomic particles. It is used to find allowed energy levels of atoms transistors. Elaboration of the equation involves partial derivatives along with vector calculus, which is beyond the scope of this manual. Nevertheless, inquisitive readers are requested to raise their quarries through *CONTACT US.*

It is an important inference of quantum mechanics that, despite wave-particle duality at a time only either particle nature can be realized or the wave nature, simultaneous realization of both the nature is not possible. In this effort to make Quantum Mechanics contextual to understanding of atomic structure, involving elaboration in previous chapter, there might abridging of concepts, inadvertently some questions on How? and Why? of involved concepts might have been left unanswered. Such questions of inquisitive readers are invited through *CONTACT US.*

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