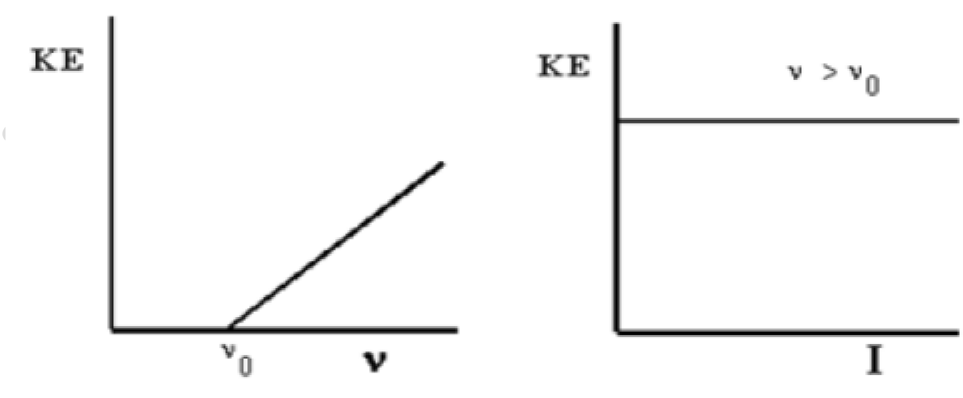
Quantum Chemistry

- **Essence of the superposition states in quantum mechanics**: The principle of quantum superposition states that if a physical system may be in one of many configurations—arrangements of particles or fields—then the most general state is a combination of all of these possibilities, where the amount in each configuration is specified by a complex number.
- **Difference between classical & quantum mechanics**: Quantum mechanics is applied to microscopic bodies whereas classical mechanics is only applicable to macroscopic bodies.
- **Photoelectric effect:** When a light radiation of suitable frequency called threshold frequency falls on a metal surface, the ejection of electrons from the metal surface take place. The ejection of electron from the surface of a metal by radiations of suitable frequency is called photoelectric effect & the ejected electrons are called photoelectrons.

  The following experimental observations were made during the experiment –

  (i) The K.E. of the ejected photoelectrons is directly proportional to the frequency of incident light.

  (ii) The K.E. of ejected photoelectrons is independent of the intensity of incident light.



(a) (b)

  (iii) No electrons are ejected from the metal unless the frequency of light used is greater than a certain minimum value, known as threshold frequency (υ_0).

  (iv) Each photon can eject one electron. It means that by increasing the intensity of light of given frequency (more than υ_0) the number of photons striking the metal surface will also increases. Hence the number of ejected electrons will increase.

Since, the light used is of a given frequency, the K.E. of the ejected electrons will remain unchanged.

- **<u>Compton shift</u>:** The scattering of $x - ray\ by$ electron & the accompanied recoiled of the particle is called Compton Effect. Compton found that if monochromatic $x - rays$ were allowed to scatter by target material such as graphite, this scattered radiations being consist of radiation of two wavelength, one having original wavelength (λ) and other having slightly longer wavelength (λ'). This phenomenon is known as Compton Effect & $\Delta\lambda = \lambda' - \lambda$ is called Compton shift. Now,

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_0 C}(1 - Cos\emptyset)$$

$$where\ \emptyset\ is\ the\ scattering\ angle.$$

<u>Compton wavelength</u>: When $\emptyset = 90^0$, i.e. the scattered radiation is perpendicular to the incident radiation, then $Cos\emptyset = 0$, so that –

$$\Delta\lambda = \frac{h}{m_0 C}(1 - 0) = \frac{h}{m_0 C} = \lambda_C$$

This is referred to as the Compton wavelength.

<u>Maximum value</u>: When $\emptyset = 180^0$, i.e. the radiation is scattered in direction opposite to the incident radiation, then $Cos\emptyset = -1$, so that –

$$\Delta\lambda = \frac{h}{m_0 C}(1 + 1) = \frac{2h}{m_0 C} = 2\lambda_C = \lambda_{max}$$

- **Does Compton shift depend on the material of the scattering? Justify your answer.**
  No, It only depends on the scattering angle. (Follow above answer)
- **Scattering of $x - rays$ by electrons in diffraction work is analogous to the Compton scattering – justify or criticize.**
  Compton effect shows the corpuscular nature of light that hits the particle causing recoiling, whereas, $x - ray$ diffraction shows the wave character of light that transcends the obstruction showing diffraction. So, the phenomena are not at all analogous. The statement is thus criticizes.
- **Photoelectric effect gives strong evidence in favor of particle nature at light. Account for the statement.**
  We know $E = h(\gamma - \gamma_0)$, if $(\gamma < \gamma_0)$, the photon will not have sufficient energy to eject electron from the metal & no photoelectric effect will be observed. As frequency (γ) increases, the K.E. of the emitted electron increases. Increase of intensity of light would mean increase the number of photons per unit volume, thereby increasing the number of electrons emitted & not their K.E. The successful explanation of experimental observation regarding photoelectric effect brought back the particle concept of light.