Atomic Physics

University of Anbar
College of Education for Pure Sciences
Department of Physics
Third Level

Dr. Waleed Subhi Al-Kubaisy

Atomic Physics

Introduction

The structure and behavior of the atom are responsible for the emergence of the virtual world. The very small distances of the atom and the properties of the nuclei require a new type, and this type is quantum mechanics, which attempts to describe the properties and behaviors of atomic and nuclear. And the development of quantum mechanics in order to be able to explain the emission and absorption of light from the atom.

The simplest type of atom is hydrogen, which consists of one electron, which orbits around the nucleus, which contains one proton.

The aim of these lectures is to understand atomic physics, as well as understanding atomic physics. It helps to study solid-state physics and astronomy, as well as its importance in many applications in medicine, communications, lasers, and others.

Theory of Relativity

The theory of relativity was discovered by the German scientist Einstein in 1905, and this theory considers the reality analysis, the speed of light in a vacuum has the same value regardless of the speed of the source or the movement of the observer. It is not possible to measure the absolute velocities, but only take the velocities in relation to the other body. The theory predicts that

$$m = \frac{m_o}{\sqrt{1-(\frac{v}{c})^2}}$$

The mass of the particle changes with the change of velocity, and according to the theory of relativity, the mass of the particle according to the above equation

$$\beta = \frac{v}{c} \qquad \gamma = \frac{1}{\sqrt{1-\beta^2}} \qquad m = \gamma m_o \qquad \gamma = \frac{m}{m_o}$$

Energy equivalence and relative mass

$$E_k = Fds \qquad F = \frac{dp}{dt} = \frac{d(mv)}{dt} \qquad v = \frac{ds}{dt}$$

$$\therefore dE_k = vd(mv) = v^2 dm + vmdv \qquad (1)$$

$$m^2 = \frac{m^2}{1 - \frac{v^2}{c^2}} = \frac{m_o^2}{\frac{c^2 - v^2}{c^2}} = \frac{m_o^2 c^2}{c^2 - v^2}$$

$$m^2 c^2 - m^2 v^2 = m_o^2 c^2$$

$$m^2 c^2 = m_o^2 c^2 + m^2 v^2 \qquad (2)$$

$$2mdmc^2 = 2mdmv^2 + 2vdvm^2 \qquad (3)$$

$$c^2 dm = v^2 dm + mvdv \qquad (4)$$

We note that equation (1) is equal to equation (4), so we get

$$dE_k = c^2 dm \qquad (5)$$

Equation (5) represents the relative change of kinetic energy with the integration of both sides

$$E_k = \int_0^{E_k} dE_k = c^2 \int_{m_o}^{m} dm = c^2 (m - m_o)$$

$$\therefore E_k = mc^2 - m_o c^2 \qquad (6)$$

$$\therefore E = mc^2 = m_o c^2 + E_k \qquad (7)$$

Where E_k is kinetic energy, $m_o c^2$ potential energy and E is total energy

$$E_k = \frac{m_o c^2}{\sqrt{1-\frac{v^2}{c^2}}} - m_o c^2 \qquad (8)$$

$$\frac{1}{\sqrt{1-\frac{v^2}{c^2}}} = \left(1-\frac{v^2}{c^2}\right)^{-1/2} = \left(1 + \frac{v^2}{2c^2} + \frac{3v^4}{8c^2} + \cdots\cdots\right)$$

$$E_k = m_o c^2 \left(1 + \frac{v^2}{2c^2} + \frac{3v^4}{8c^2} + \cdots\cdots\right)$$

To find the relationship between the body's total energy and momentum, we multiply equation (2) by c^2 to get

$$E^2 = p^2 c^2 + m_o c^4 \qquad E = mc^2 = m_o c^2 + E_k$$

$$E^2 = m_o^2 c^4 + 2m_o c^2 E_k + E_k^2$$

$$\therefore p = \sqrt{2m_o E_k + \frac{E_k^2}{c^2}}$$

The second term is called the correction term

Example: An electron has a potential energy of 0.511 MeV and a kinetic energy of 200 keV. Find the speed of its velocity

Solution

$$E = mc^2 = m_o c^2 + E_k$$

$$\frac{m_o c^2}{\sqrt{1-\frac{v^2}{c^2}}} = m_o c^2 + E_k \qquad \gamma m_o c^2 = m_o c^2 + E_k$$

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$$\gamma = 1 + \frac{E_k}{m_o c^2} \qquad \gamma = 1 + \frac{200}{511} = 1 + 0.391 = 1.391$$

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{1}{\sqrt{1 - \beta^2}} \qquad \beta^2 = \sqrt{1 - \frac{1}{\gamma^2}} = 0.695$$

$$\beta = \frac{v}{c} \Rightarrow v = \beta c = 0.695 \times 3 \times 10^8 = 2.085 \times 10^8 \, m/\sec$$

Example \ What is the kinetic energy of a neutron with a velocity of 6×10^7 m/sec where $m_n = 939.55$ MeV

<u>Solution</u>

$$\beta = \frac{v}{c} = \frac{6 \times 10^7}{3 \times 10^8} = 0.2 \qquad E_k = (\gamma - 1)m_o c^2 = \left(\frac{1}{\sqrt{1 - \beta^2}} - 1 \right) m_o c^2$$

$$(1.021 - 1)939.55 = 19.73 MeV$$

Black Body Radiation

Many scientists tried to discover the basic laws of thermal radiation based on properties that were known, the most important of which is

1- The body becomes glowing with increasing temperature, and the amount of radiation emitted also changes with the change in temperature

2- The color of the emission changes with increasing temperature. For example, if a piece of iron is heated, we notice a gradual change in its color from dark, red, orange and yellow to white.

If a shiny metal particle is taken and a light is shined on it, it will reflect almost all the light falling on the metal piece, but if this light falls on a black body, it will absorb all the light and may not be reflected from it at all.

Through this experiment, scientists drew attention to the black body, since it absorbs all radiation, so it heats up at a higher temperature than the other body if it is exposed to the same temperature. But if it is considered as a source of light radiation, its intensity will be greater if it is raised to the same temperature in relation to the other body.

The scientists chose a hollow sphere with a small hole in it and its inner walls covered with black marble. If radiation enters through the hole, whatever its wavelength is, it is absorbed by the inner walls after suffering many reflections.

The black body absorbs all wavelengths. When the temperature of the ball is raised regularly, it will emit radiation through the small hole containing all wavelengths.
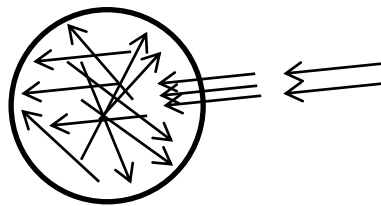
If we draw a graph of the spectrum of the thermal emissions of a black body at different temperatures between energy and wavelength, after taking a narrow beam from a hot body and passing it through a special spectrometer to sort its waves, the radiant energy in this beam is measured with a special thermometer, and we notice from the drawing

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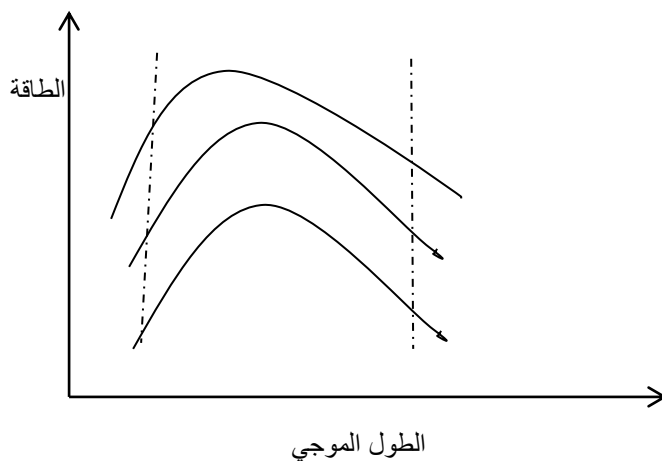
1- Energy starts from zero when the wavelength is zero and approaches zero at infinity
2- The maximum limit lies between these two values
3- The upper end of the two curves rises as the temperature rises and shifts towards short wavelengths.

Question: Why don't all bodies radiate their internal energy to the end and cool down to absolute zero?

The answer to this is that the reason for this is due to the environment, if we assume the presence of the body inside the room so that the walls of the room and the rest of the existing bodies radiate this energy and intercept the body and absorb and transform into internal energy. If the body is at a temperature greater than room temperature, the body will start In transmitting its heat to the ocean.

An example of this is an electric lamp equipped with electrical power. It will convert its electrical energy into light energy and transmit it to the ocean, given that the time rate of emission is greater than the time rate of absorption, and it is in a state of equilibrium if the time rate of absorption is equal to the time rate of emission.

Suppose there are several opaque bodies whose absorbance is a_1, a_2, a_3, ……. and reflectivity r_1, r_2, r_3, ……… they are in equilibrium with each other and with the surroundings. If a ray of small wavelength and intensity falls, a large part of the radiation will be absorbed by the body and a small part will be reflected, so the sum of the rate of reflection and absorption of the body is equal to one

$a_1+r_1=1$

Radiation intensity I Emission power for wavelength w_λ , First body area ΔA_1 Total radiance in the case of emission

$$w_1\Delta A_1\Delta t \tag{1}$$

body absorption

$$a_1 I\, \Delta A_1 \Delta t \qquad\qquad (2)$$

in equilibrium

$$w_1 \Delta A_1 \Delta t = a_1 I\, \Delta A_1 \Delta t \qquad\qquad (3)$$

$$w_2 \Delta A_2 \Delta t = a_2 I\, \Delta A_2 \Delta t \qquad\qquad (4)$$

And by dividing (3) by (4)

$$\frac{w_1}{a_1} = \frac{w_2}{a_2} \qquad\qquad (5)$$

$$\frac{w_1}{w_2} = \frac{a_1}{a_2} \qquad\qquad (6)$$

And if a for a black body is equal to one

$$\therefore \frac{w_1}{w_2} = 1 = w_b$$

Suppose we have a cavity in the form of two parallel plane plates of two different materials and that the ray travels back and forth between the two planes at equal temperature

emitter M_2	emitter M_1
$W_1\Delta t \rightarrow$ to (2)	(1) to $\leftarrow W_2\Delta t$
$(1-a_2)\, W_1\Delta t \leftarrow$	$(1-a_1)\, W_2\Delta t \rightarrow$
$(1-a_1)(1-a_2)\, W_1\Delta t \rightarrow$	$(1-a_1)(1-a_2)\, W_2\Delta t \leftarrow$
$(1-a_1)(1-a_2)^2\, W_1\Delta t \leftarrow$	$(1-a_1)^2(1-a_2)\, W_2\Delta t \rightarrow$
$(1-a_1)^2(1-a_2)^2\, W_1\Delta t \rightarrow$	$(1-a_1)^2(1-a_2)^2\, W_2\Delta t \leftarrow$
$(1-a_1)^2(1-a_2)^3\, W_1\Delta t \leftarrow$	$(1-a_1)^3(1-a_2)^2\, W_2\Delta t \rightarrow$

The radiation lines emitted from the unit area of each face through a period of time Δt in order for the beam to cross between two parallel plates, meaning that the radiation will fall on the first face and lose its energy and reflect part of another of it and through the occurrence of these successive passes of the first radiation from each face until the arrival of To stabilize it will pass through the tunnel and towards the right.

$$w_r \Delta t = w_1 \Delta t + (1-a_1)(1-a_2)w_1 \Delta t + (1-a_1)^2(1-a_2)^2 w_1 \Delta t + \ldots\ldots$$
$$+ (1-a_1)w_2 \Delta t + (1-a_1)^2(1-a_2)w_2 \Delta t + (1-a_1)^3(1-a_2)^2 w_2 \Delta t \ldots\ldots \tag{7}$$

Let $\quad x = (1-a_1)(1-a_2)$

$$w_r = w_1(1 + x + x^2 + \ldots\ldots) + w_2(1-a_1)(1 + x + x^2 + \ldots\ldots) \tag{8}$$

$$\frac{1}{1-x} = \frac{1}{1-(1-a_1)(1-a_2)} = \frac{1}{1-(1-a_1-a_2+a_1a_2)} = \frac{1}{a_1+a_2-a_1a_2} \tag{9}$$

$$w_2 = a_2 w_b$$
$$w_1 = a_1 w_b \tag{10}$$

$$w_r = \frac{a_1 w_b + a_2 w_b(1-a_1)}{a_1+a_2-a_1a_2} = \frac{w_b(a_1+a_2-a_1a_2)}{a_1+a_2-a_1a_2} = w_b \tag{11}$$

It has been experimentally proven by the scientist Stellan and theoretically by the scientist Boltzmann that the radiant energy per unit time E of the radiating black body is proportional to the absolute temperature T^4

$$E \propto T^4 \qquad E = \sigma T^4$$

Where σ is Boltzmann's constant and is equal to $\sigma = (5.6696 \pm 0.001) * 10^{-8}$ wat.m^{-2}.k^{-4}

The total energy emitted per unit time of the emitting area is proportional to the area under the curve.

Explanation of the reasons for the black body radiation and the reason for the continuity of its spectrum and its dependence on temperatures.

1- Finn: His attempts were, according to classical physics, all bodies contain electrical charges such as electrons and protons, and in temperatures these charges fluctuate rapidly and increase as the temperature rises. a certain temperature.

Fenn developed an interpretation of the heat radiation energy distribution curve, and his theory succeeded with the experimental curve, but it failed at large wavelengths.
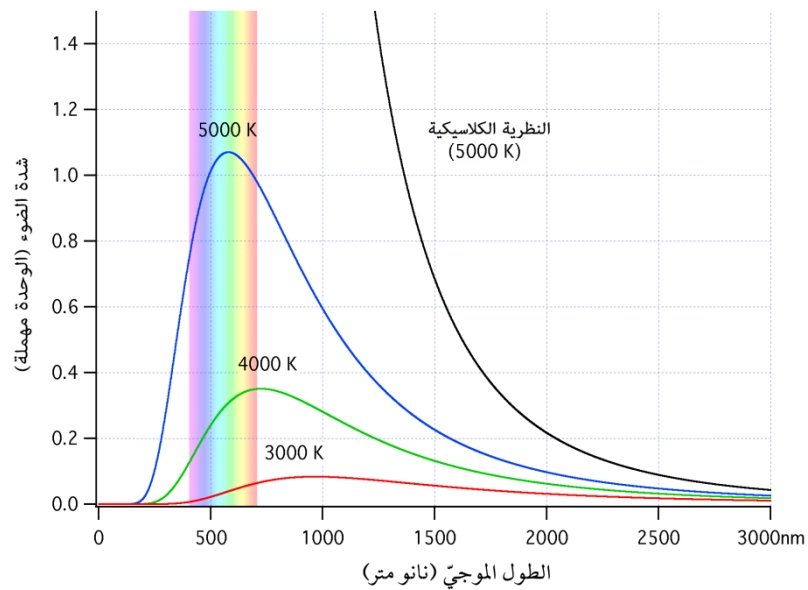
$$\lambda_{max} = \frac{b}{T}$$

2- Riley-Jeans's Trying
   The black body was discussed, where the thermal rays are reflected at the inner walls of the black body gap back and forth forming stable waves for each frequency. Experimental radiative curves

$$F(\lambda) = \frac{2\pi ckT}{\lambda^4}$$

c is speed of light

k is Boltzmann's constant

As the wavelength decreases, it continues to rise until it reaches its maximum limit and then begins to decline, but according to Rayleigh-Jones law, the intensity of heat radiation increases as the wavelength shortens and continues to rise to infinity.

3- Plank's Trying

There are two equations equation that agree with high frequencies and fail with low frequencies, while the other equation agrees with low frequencies and fails with high frequencies.

Since the charges fluctuate at all possible frequencies and energies, continuous electromagnetic waves are expected to cover the spectrum of the black body. on the continuity of electromagnetic waves. Planck assumed that radiation of frequency (γ) is emitted and absorbed in the form of quanta

0, hγ, 2hγ, ……………

h= 6.62*10^{-34} J.s   blank's constant

The amount of violet light is greater than the frequency of red light. When the oscillator moves from one energy to another or from bottom to top, it absorbs energy, ie, moving from the lower level to the higher level.

The effect of radiation on matter

Radiation affects the material in three ways, depending on the energy of the radiation falling on the material, and these methods are:

1- The effect of the photoelectric phenomenon
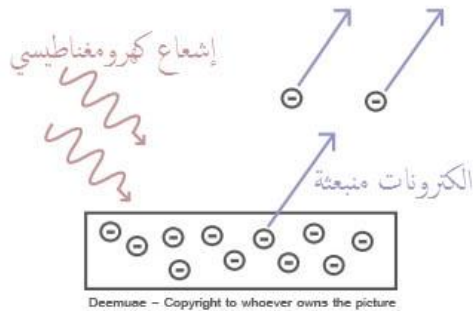
$$p_\gamma = p_\alpha + p_e \qquad\qquad (1)$$

$$E_\gamma = T_e + T_\alpha + E_B$$

$$E_\gamma = T_e + E_B \qquad\qquad T_e = E_\gamma - E_B$$

 Where E_γ and p_γ are the energy and momentum of the incident radiation, respectively, T_e and p_e are the kinetic energy and momentum of the liberated electron, E_B, the energy of the electron's attachment to the atom, and P_α the atom's recoil momentum.

The probability of the occurrence of the photoelectric phenomenon when the energy of a photon ranges from 0.1 to half a million electron volts. The kinetic energy plus the recoil energy of the atom plus the bonding energy. The recoil energy can be neglected because it is small.

$$\boxed{T_e = h\upsilon - E_B}$$

The photoelectric phenomenon can occur in other orbitals, such as M and L, and so if the incident energy is less than the bonding energy of the electron in the M orbital, it will move to the other orbit, as shown in the following figure

| L=	0	1	2	3	4	5	6	7	8	9	10	11
symbol	s	p	d	f	g	h	I	k	L	M	N	o

L is the total angular momentum
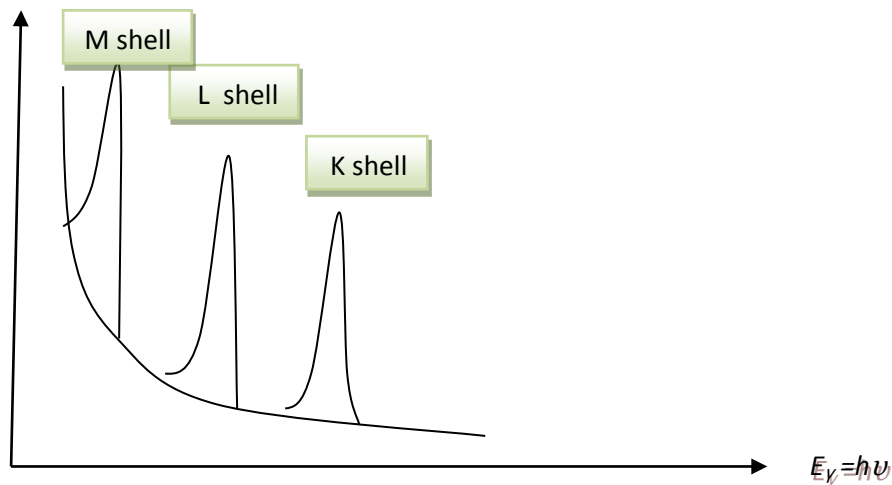
When the gamma rays exceed half a million electron volts, the photoelectrons are emitted from the k orbital.

According to Maxwell's theory, the speed of electrons increases with the increase in the intensity of the incident rays, but the result is different as the number of electrons increases with the increase in the incident intensity, meaning that the number of emitted electrons per second is directly proportional to the incident intensity and the speed of electrons increases with the increasing frequency of the incident rays, and there is a limit for the emission of electrons called the threshold limit without that An electron cannot separate from an atom.
The following figure shows the practical experiment on the occurrence of the photoelectric phenomenon
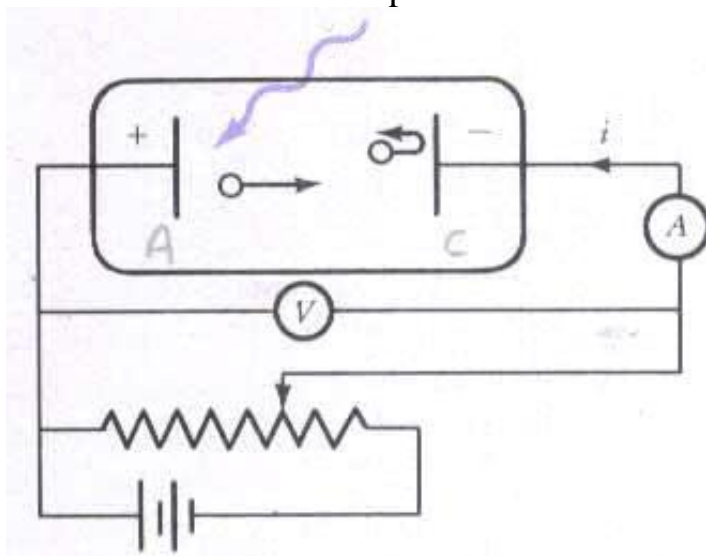
When a monochromatic electromagnetic beam falls on the surface of the metal anode connected to the positive terminal of the battery and is inside an airless container, to prevent the collision of freed electrons with air molecules. When the electrons are liberated from the surface of the metal and are able to reach the negative plate and the cathode, and most of the time it is of the same material as the anode, an electric current passes in the circuit and can be measured through the ammeter, which expresses the intensity of the photovoltaic current passing through the circuit and the greater the number of electrons liberated from the surface of the metal The higher the output current. Note here that the direction of the conventional current is in the opposite direction of the movement of electrons.

Note that

1- The energy of the electrons released from the anode is different
2- The electric force generated by the electric field between the cathode and the anode acts in the opposite direction of the electrons' movement.
3- The kinetic energy of the electrons is equal to the work done on them by the electric field through the following relationship: $1/2mv^2=eV$

To measure the kinetic energy of the electrons, it is by slowing and stopping the electrons, and this is done by reversing the polarities of the voltage applied to the two plates until it reaches a reading of zero.

Example \ If the threshold frequency of sodium is 4.4 * 10^{14} Hz (1) what is the energy done to free an electron (2) If the frequency of the incident light is 10^{15} Hz, what is the greatest kinetic energy that the photon gives to the electron

Solution\

$$E = h\upsilon = 6.62 \times 10^{-34} J.s \times 4.4 \times 10^{14} \sec^{-1} = 2.9 \times 10^{-19} joule$$

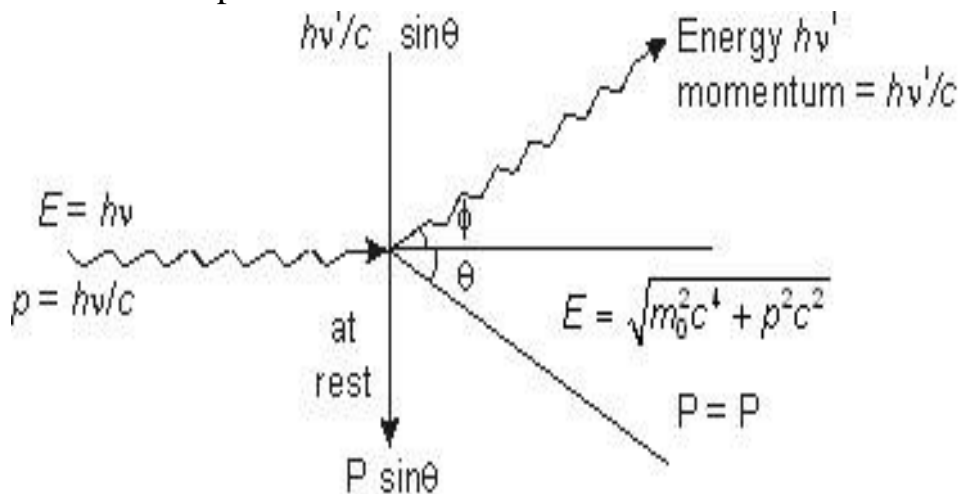$$h\upsilon = 6.62 \times 10^{-34} J.s \times 10^{15} \sec^{-1} = 6.6 \times 10^{-19} joule$$

$$T_e = h\upsilon - E_B = 6.6 \times 10^{-19} - 2.9 \times 10^{-19} = 2.3 eV$$

Example \ What is the energy of an infrared photon if its wavelength is 10^{-6}

2- Compton effect

When the energy of the photon is greater than a certain amount of the correlation energy, an inelastic collision of the rays with the electron can occur, where we notice that after the fall of the photon and its collision with the electron, it is scattered at an angle θ and the photon is scattered at an angle ϕ and υ represents the frequency of the incident photon and ῡ represents the frequency of the scattered photon

$$T_e = h\upsilon - h\upsilon' \tag{1}$$

$$E = h\upsilon = pc \qquad h = p\lambda \Rightarrow \lambda = \frac{c}{\upsilon}$$

$$p = \frac{h\upsilon}{c} \tag{2}$$

$$\frac{h\upsilon}{c} = \frac{h\upsilon'}{c}\cos\phi + p\cos\theta \tag{3}$$

$$pc\cos\theta = h\upsilon - h\upsilon'\cos\phi \tag{4}$$

$$\frac{h\upsilon'}{c}\sin\phi = p\sin\theta \Rightarrow pc\sin\theta = h\upsilon'\sin\phi \qquad (5)$$

By squaring equations (4) and (5) and adding them together, we get

$$p^2c^2 = (h\upsilon)^2 - 2(h\upsilon)(h\upsilon')\cos\phi + (h\upsilon')^2 \qquad (6)$$

It is known that total energy = kinetic energy + potential energy

$$E = m_o c^2 + T_e \qquad (7)$$

m$_o$ is the rest mass of the body, and the total energy is defined by Dirac's assumption

$$E = \sqrt{m_o^2 c^4 + p_e^2 c^2} \qquad (8)$$

$$(m_o c^2 + T_e)^2 = m_o^2 c^4 + p_e^2 c^2$$
$$m_o^2 c^4 + 2m_o c^2 T_e + T_e^2 = m_o^2 c^4 + p_e^2 c^2$$
$$p_e^2 c^2 = T_e^2 + 2m_o c^2 T_e \qquad (9)$$

$$T_e = h\upsilon - h\upsilon'$$
$$T_e^2 = (h\upsilon)^2 - 2(h\upsilon)(h\upsilon') + (h\upsilon')^2 \qquad (10)$$

In compensation (9) and (10)

$$p_e^2 c^2 = (h\upsilon)^2 - 2(h\upsilon)(h\upsilon') + (h\upsilon')^2 + 2m_o c^2 (h\upsilon - h\upsilon') \qquad (11)$$

Substituting pc into equation (6) in (11) we get

$$(h\upsilon)^2 - 2(h\upsilon)(h\upsilon')\cos\phi + (h\upsilon')^2 = (h\upsilon)^2 - 2(h\upsilon)(h\upsilon')$$
$$+(h\upsilon')^2 + 2m_oc^2\left(h\upsilon - h\upsilon'\right)$$

$$\therefore 2m_oc^2\left(h\upsilon - h\upsilon'\right) = 2(h\upsilon)(h\upsilon')(1-\cos\phi) \qquad (12)$$

And by dividing by $2c^2h^2$

$$\frac{m_oc}{h}\left(\frac{\upsilon}{c} - \frac{\upsilon'}{c}\right) = \frac{\upsilon\upsilon'}{c^2}(1-\cos\phi) \qquad (13)$$

$$\frac{m_oc}{h}\left(\frac{1}{\lambda} - \frac{1}{\lambda'}\right) = \frac{(1-\cos\phi)}{\lambda\lambda'} \qquad (14)$$

$$\lambda' - \lambda = \frac{h}{m_oc}(1-\cos\phi) \qquad (15)$$

$$\Delta\lambda = \frac{h}{m_oc}(1-\cos\phi)$$

And by moving 1/υ and dividing by h and λ=c/υ

$$\frac{1}{h\upsilon'} - \frac{1}{h\upsilon} = \frac{1}{m_oc^2}(1-\cos\phi)$$

$$\boxed{\therefore h\upsilon' = \frac{h\upsilon}{1 + \frac{h\upsilon}{m_oc^2}(1-\cos\phi)}} \qquad (16)$$

Let $\quad \alpha = \dfrac{h\upsilon}{m_oc^2} \qquad\qquad h\upsilon'_{\max} = h\upsilon \Rightarrow \cos\phi = 1 \Leftrightarrow \phi = 0$

$$h\upsilon'_{\min} = \frac{h\upsilon}{1+2\alpha} \qquad\qquad when \quad \phi=180^o$$

$$T_e = h\upsilon - \frac{h\upsilon}{1+\alpha(1-\cos\phi)} \Rightarrow T_e = h\upsilon\frac{\alpha(1-\cos\phi)}{1+\alpha(1-\cos\phi)}$$

Example: A photon with an energy of 3 million electron volts falls and the Comten phenomenon occurs. Find the energy of the photon and the energy of the scattered electron at 90° and 180° static energy (moc2=0.511MeV).

Solution

$$E'_\lambda = h\upsilon' = \frac{h\upsilon}{1+\dfrac{h\upsilon}{m_o c^2}(1-\cos\phi)} = \frac{3}{1+\dfrac{3}{0.511}(1-0)} = 0.437 MeV$$

$$T_e = h\upsilon - h\upsilon' = 3 - 0.437 = 2.503 MeV$$

3- **Pair production**

In the case of absorbing energy equal to twice the rest mass of the electron (0.511 MeV), a pair of electron and positron equal to

$2m_o c^2 = 1.02 MeV$

So Dirac's electron equation solved this problem, and Dirac assumed that the electron could exist in one of the two energy levels.

1- It has a wave energy and a rest mass of $m_o c^2$, so the energy of the electron is either greater or equal to $m_o c^2$.

$E \geq moc2$

2- A level with negative energy $m_o c^2$ so that $E \leq m_o c^2$ The area between them is called the non-permissible field

Atomic Model

1- Thomson Model

 In lesson 3 you have learnt that all matter is made of atoms and all the atoms are electrically neutral. Having discovered electron as a constituent of atom, Thomson concluded that there must be an equal amount of positive charge present in an atom. On this basis he proposed a model for the structure of atom. According to his model, atoms can be considered as a large sphere of uniform positive charge with a number of small negatively charged electrons scattered throughout it, Fig. 5.4. This model was called as plum pudding model. The electrons represent the plums in the pudding made of negative charge. This model is similar to a water-melon in which the pulp represents the positive charge and the seeds denote the electrons. However, you may note that a water melon has a large number of seeds whereas an atom may not have as many electrons.
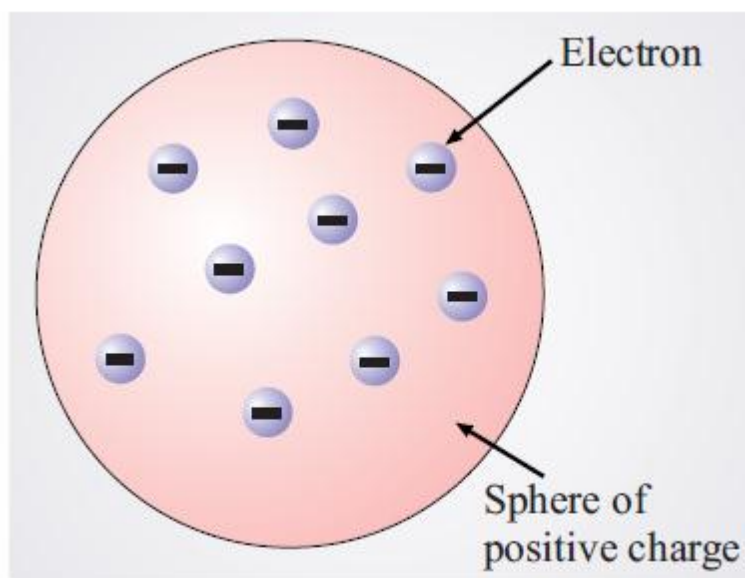
2- Rutherford's model

Ernest Rutherford and his co-workers were working in the area of radioactivity. They were studying the effect of alpha (α) particles on matter. The alpha particles are helium nuclei, which can be obtained by the removal of two electrons from the helium atom. In 1910, Hans Geiger (Rutherford's technician) and Ernest Marsden (Rutherford's student) performed the famous α-ray scattering experiment. This led to the failure of Thomson's model of atom. Let us learn about this experiment. α-Ray scattering experiment In this experiment a stream of α particles from a radioactive source was directed on a thin (about 0.00004 cm thick) piece of gold foil. On the basis of Thomson's model it was expected that the alpha particles would just pass straight through the gold foil and could be detected by a photographic plate placed behind the foil. However, the actual results of the experiment, Fig., were quite surprising. It was observed that:

(i)   Most of the α-particles passed straight through the gold foil.
(ii)   Some of the α-particles were deflected by small angles.
(iii)   A few particles were deflected by large angles.
(iv)   About 1 in every 12000 particles experienced a rebound
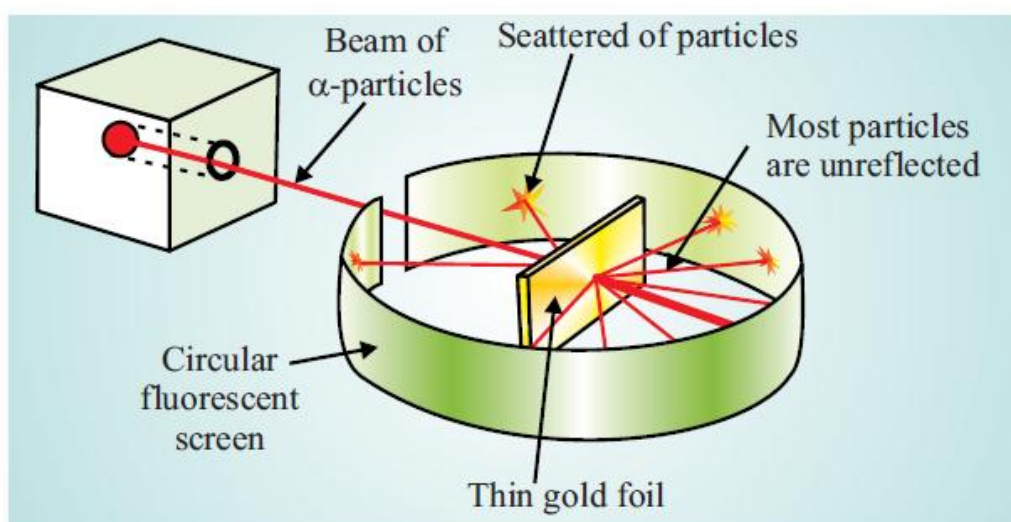
The results of α-ray scattering experiment were explained by Rutherford in 1911 and another model of the atom was proposed. According to Rutherford's model, Fig. 5.6(a).

a- An atom contains a dense and positively charged region located at its centre; it was called as nucleus,

b- All the positive charge of an atom and most of its mass was contained in the nucleus,

c- The rest of an atom must be empty space which contains the much smaller and negatively charged electrons,

(a)   (b)
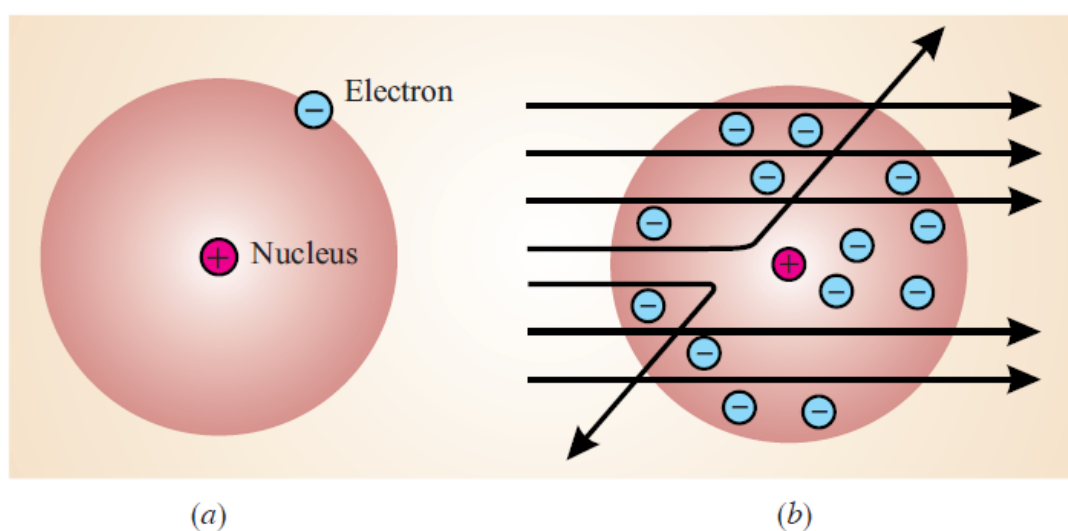
On the basis of the proposed model, the experimental observations in the scattering experiment could be explained. This is illustrated in Fig. above. The α particles passing through the atom in the region of the electrons would pass straight without any deflection. Only those particles that come in close vicinity of the positively charged nucleus get deviated from their path. Very few α-particles, those that collide with the nucleus, would face a rebound. On the basis of his model, Rutherford was able to predict the size of the nucleus. He estimated that the radius of the nucleus was at least 1/10000 times smaller than that of the radius of the atom. We can imagine the size of the nucleus with the following analogy. If the size of the atom is that of a cricket stadium then the nucleus would have the size of a fly at the centre of the stadium.

3- BOHR'S MODEL OF ATOM

In 1913, Niels Bohr,a student of Rutherford proposed a model to account for the shortcomings of Rutherford's model. Bohr's model can be understood in terms of two postulates proposed by him. The postulates are: Postulate 1: The electrons move in definite circular paths of fixed energy around a central nucleus; just like our solar system in which different planets revolve around the Sun in definite trajectory. Similar to the planets, only certain circular paths around the nucleus are allowed for the electrons to move. These paths are called orbits, or energy levels. The electron moving in the orbit does not radiate. In other words, it does not lose energy; therefore, these orbits are called stationary orbits or stationary states. The bold concept of stationary state could answer the problem of stability of atom faced by Rutherford's model.
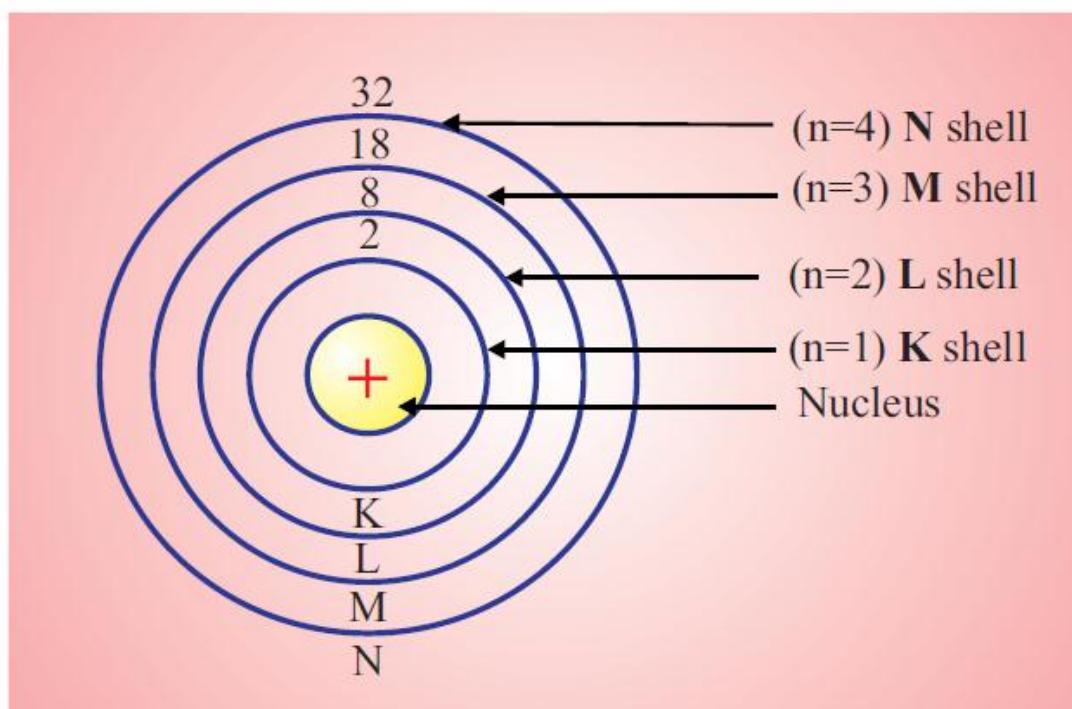
It was later realised that the concept of circular orbit as proposed by Bohr was not adequate and it was modified to energy shells with definite energy. While a circular orbit is two dimensional, a shell is a three dimensional region. The shells of definite energy are represented by

letters (K, L, M, N etc.) or by positive integers (1, 2, 3, …. etc.) Fig.. The energies of the shells increase with the number n; n = 1,

level is of the lowest energy. Further, the maximum number of electrons that can be accommodated in each shell is given by 2n2, where n is the number of the level. Thus, the first shell (n=1) can have a maximum of two electrons whereas the second shell can have 8 electrons and so on. Each shell is further divided into various sublevels called subshells about which you would study in your higher classes. Postulate 2: The electron can change its shells or energy level by absorbing or releasing energy. An electron at a lower state of energy Ei can go to a final higher state of energy Ef by absorbing a single photon of energy given by: $E = h\nu = E_f - E_i$ Similarly, when electron changes its shell from a higher initial level of energy Ei to a lower final level of energy Ef , a single photon of energy $h\nu$ is released (Fig.).
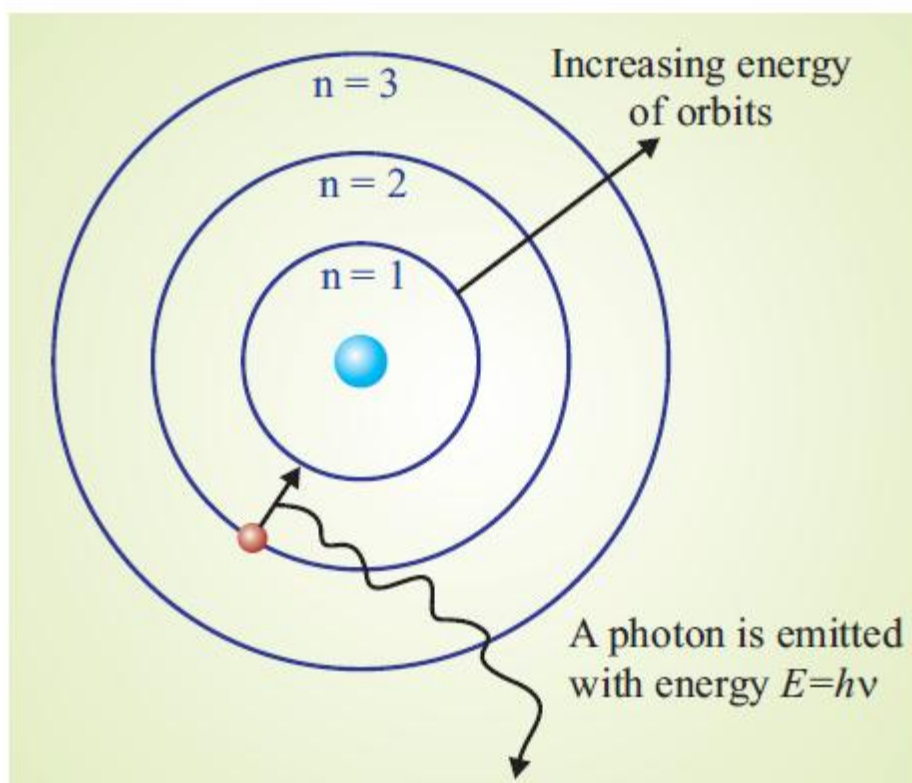
For the purpose of calculating the permissible orbits predicted by the scientist Bohr, he used the hydrogen atom, which consists of one positive charge around which one electron revolves, and assume that the nucleus is fixed and that the electron revolves around the nucleus with a radius of r.

$$Q = -Ze = -e \qquad (1)$$

Z is atomic number, Q is the total charge

Bohr used Newton's second law and Coulomb's law

$$f = ma \qquad (2)$$

$$a = \frac{v^2}{r}$$

$$f = \frac{(-Ze)e}{4\pi\varepsilon_o r^2} \qquad (3)$$

$$f = -k\frac{e^2}{r^2} \qquad (4)$$

v is electron velocity

$$\therefore -k\frac{e^2}{r^2} = -m\frac{v^2}{r}$$

$$mv^2 = k\frac{e^2}{r} \qquad (5)$$

One of Bohr's hypotheses is that in order for an electron to orbit in one of the orbits, it must have an angular momentum of multiples $n\hbar$

$$L = mvr = n\hbar = n\frac{h}{2\pi} \qquad (6)$$

$$\therefore v = \frac{nh}{2\pi mr} \Rightarrow\Rightarrow v^2 = \frac{n^2h^2}{4\pi^2m^2r^2} \qquad (7)$$

From equation (5)

$$v^2 = \frac{ke^2}{rm} \qquad (8)$$

And equal to equations (7) and (8), we get

$$\frac{ke^2}{rm} = \frac{n^2h^2}{4\pi^2m^2r^2}$$

$$ke^2 = \frac{n^2h^2}{4\pi^2mr}$$

$$\boxed{\therefore r = \frac{n^2h^2}{4\pi^2mke^2}} \qquad (9)$$

The total energy according to the Bohr model

The total energy is the sum of kinetic energy + potential energy

$$E = T + V \qquad (10)$$

$$T = \frac{1}{2}mv^2$$

And from the Bohr model of equation (5) we have

$$mv^2 = k\frac{e^2}{r}$$

$$T = \frac{ke^2}{2r} \qquad (11)$$

The potential energy at a distance r from the charge Q is

$$k\frac{Q}{r}$$

$$k\frac{Q}{r} = k\frac{(Ze)e}{r}$$

$$\therefore V = \frac{-ke^2}{r} \qquad (12)$$

So the total energy is

$$E = \frac{ke^2}{2r} + \left(\frac{-ke^2}{r}\right) \Rightarrow\Rightarrow E = -\frac{ke^2}{2r} \qquad (13)$$

$$\therefore r = -\frac{ke^2}{2E} \qquad (14)$$

By equating the two equations (14) with (9), we get

$$-\frac{ke^2}{2E} = \frac{n^2 h^2}{4\pi^2 mke^2}$$

$$E = -\frac{2\pi^2 mk^2 e^4}{n^2 h^2} \qquad\qquad k = \frac{1}{4\pi\varepsilon_o}$$

$$E = -\frac{2\pi^2 me^4}{16\pi^2 \varepsilon_o^2 n^2 h^2} \qquad\qquad \boxed{\therefore E = -\frac{me^4}{8\varepsilon_o^2 n^2 h^2}}$$

Putting Z back into the equation, we get

$$E = -\frac{Z^2me^4}{8\varepsilon_0^2n^2h^2}$$

Substituting for the constants, we get the energy in electron volts.

$$E = -\frac{13.6}{n^2}ev$$

We note from this equation that the energy is inversely proportional to the square of the main orbital number (n), and the negative sign indicates an effort to free the electron from attracting the nucleus. The energy level (n = 1) represents the ground state and the stable state, while n = 2, 3, 4, … It refers to the unstable levels. If the quantum number approaches infinity, this means that the energy of the levels approaches zero and the energy of the electron becomes zero. The electron in this case is free and not restricted by the electric field of the nucleus. The energy required to remove an electron from the ground level to the infinity level is known as the ionization potential.

The ionization potential of a hydrogen atom is (13.6 eV)

$$n = 1 \Rightarrow E_1 = -\frac{13.6}{1^2} = -13.6ev$$

$$n = 2 \Rightarrow E_2 = -\frac{13.6}{2^2} = -3.4ev$$

$$n = 3 \Rightarrow E_3 = -\frac{13.6}{3^2} = -1.5ev$$

$$n = 4 \Rightarrow E_4 = -\frac{13.6}{4^2} = -0.8ev$$

$$n = \infty \Rightarrow E_\infty = -\frac{13.6}{\infty^2} = 0$$

Calculating the radii of electronic orbits

$$r = \frac{n^2 h^2}{4\pi^2 m k e^2}$$

Orbit radius n = 1 (smallest orbit) after compensation

$$r = a_o = 0.529 \times 10^{-10} m = 0.529 A^o$$

According to Bohr's second assumption, orbitals have specific energies, so the transfer of an electron from one orbit to another will be accompanied by gain or loss of energy.

$$\upsilon = \frac{E_i - E_f}{h} \qquad\qquad E_n = -\frac{k^2 2\pi^2 m e^4}{n^2 h^2}$$

n_i represents the initial orbital and n_f represents the final orbital

$$\upsilon = \frac{k^2 2\pi^2 m e^4}{h^3}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

$$k' = \frac{1}{\lambda} = \frac{\upsilon}{c}$$

K' is the wave number, and to write the equation in terms of the wave number k'

$$k' = \frac{k^2 2\pi^2 m e^4}{c h^3}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

$$k' = R_H \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

R_H is the Rydberg constant

There are five series of hydrogen spectral lines

1- Lyman series: The result of the electron transition from n>1 to n=1 . is produced

$$k' = R_H \left(\frac{1}{1^2} - \frac{1}{n_i^2} \right)$$ n_i=2, 3 ,4 ....

3- Palmer series: - We get it from the transition of an electron from n>2 to n=2

$$k' = R_H \left(\frac{1}{2^2} - \frac{1}{n_i^2} \right)$$ n_i=3, 4, 5...........

4- Paschen series:- We get it from the transition of an electron from n>3 to n=3

$$k' = R_H \left(\frac{1}{3^2} - \frac{1}{n_i^2} \right)$$ n_i=4, 5, 6...........

5- The Brackett series: We get it from the transition of an electron from n>4 to n=4

6- Pfond series: - We get it from the transition of an electron from n>5 to n=5

Example/ Calculate the wavelength of the photon emitted when a hydrogen atom moves from n=3 to n=2.

X-Rays: transitions involving inner shell electrons

We have been concerned, so far, with the energy levels of the valence electrons i.e. those electrons outside the filled shells (or sub-shells). Transitions between these levels involve photons in the energy range of _ 10eV down to 10^{-6}eV. These energies correspond to wavelengths of _ 10^{-7}m to 1m. (Ultra Violet, visible, infra-red, microwaves and radio waves). When photon energies are much larger than 10eV i.e. in the keV range then the interaction can disturb the tightly bound, inner-shell electrons. Conversely, transitions of an inner-shell electron from one shell

to another will involve emission or absorption of the high energy, short-wavelength photons; X-rays. Usually, however, all the energy

levels of the inner shells are occupied, so, in order to allow transitions to occur at all, we first have to create a vacancy in one of the inner shells. The energy required to do this can come from either the absorption of a sufficiently energetic photon, or from the kinetic energy of impact with a high energy electron.

X-ray Spectra

X-rays are generated when high energy electrons strike a solid target e.g. the metal anode in a "cathode-ray" tube. The spectrum of the X-rays generated in this way consists firstly of a continuous

range of wavelengths down to a limiting value corresponding to the maximum energy of the incident electrons. These X-rays are the result of the deceleration of the charged particles and are known as "bremsstrahlung" or "braking radiation".
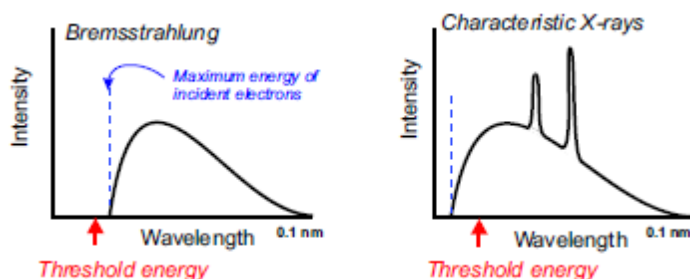
When the energy of the electrons is increased above a certain value, for a given target material, sharp peaks i.e. discrete lines, appear superimposed on the continuous "bremsstrahlung". The

spectrum of these discrete lines are characteristic of the target element. These characteristic X-rays have the following properties:

• The wavelengths fit a simple series formula.

• All the lines of a particular series appear together once the incident electrons exceed a particularthreshold energy.

• The threshold energy for a particular series just exceeds the energy of the shortest wavelength in the series.

• Above a certain energy, no new series appear.

These observations are explained by the following process:

The incident energy (from electron impact) is transferred to an inner-shell electron. If this energy is sufficient the inner-shell electron is raised to a vacant energy level. Now the vacancy energy levels are those lying between the atoms ground state energy and the ionization limit. This is a range of only 10eV or so. If the incident energy is of the order of 103eV, or greater, then the most likely result is to ionize the atom i.e. the inner-shell electron escapes with a kinetic energy equal to the incident impact energy less the binding energy of the inner shell. An electron from a higher inner shell may "fall" into the vacancy. As a result of this transition an X-ray photon is emitted with an energy corresponding to the difference in binding energy of the two shells. For example, creation of a vacancy in the n = 3 shell allows electrons from n = 4, or higher shells to "fall" into the n = 3 vacancy. (Higher energy impacts may eject electrons from deeper shells n = 2 and n = 1) These transitions are the source of the discrete, characteristic, X-ray lines. X-ray spectroscopy developed its own nomenclature and it is still (unfortunately) used, so we have to live with a further set of labels. In the context of X-rays the n = 1, 2, 3 shells are knows as K, L, M etc. respectively.

X-ray series

The X-rays emitted in transitions between inner-shell energy levels will have energies corresponding to the difference in binding energy of the electrons in the two shells concerned. The binding energy of an electron in a given shell of quantum number, n, may be expressed using a hydrogenic model:

$$E_n = \frac{R(Z - \sigma_n)^2}{n^2}$$

Where R is Rydberg's constant. _n is a screening factor that accounts for the effect of the other electrons.

For the K-shell (n = 1) there are 2 electrons. As the ejected electron moves outwards the remaining electron provides a spherically symmetric shell around the nucleus of Z protons and reduces the effective nuclear charge to (Z − 1). The other electrons in higher shells also make a contribution to the screening. The total screening factor, _k is then approximately 2. It is difficult to calculate screening factors, although good estimates can be made using atomic structure calculations. Usually we reply on experimental (empirical) values for _. (The screening factors also depend on the angular momentum of the states involved.) Transitions from higher shells to a vacancy in the K-shell give rise to a series of lines. The wavenumber (_ = 1/_) of these lines will be given by the differences in the binding energies:

K-series:
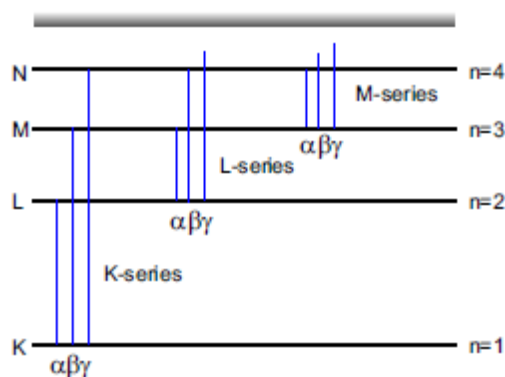
$$\bar{\nu}_K = R\left\{ \frac{(Z - \sigma_K)^2}{1^2} - \frac{(Z - \sigma_i)^2}{n_i^2} \right\}$$

Where ni = 2, 3, 4 etc.

In general:

$$\bar{\nu}_X = R\left\{ \frac{(Z - \sigma_i)^2}{n_i^2} - \frac{(Z - \sigma_j)^2}{n_j^2} \right\}$$

With n_i, n_j integers and $n_i < n_j$.

The longest wavelength series member is labelled _, with successive lines denoted _, etc.

Fine structure of X-ray spectra

A single vacancy in an otherwise full shell has the properties of a single electron in an otherwise empty shell. The X-ray energy levels therefore resemble those of hydrogen or alkali atoms. The energy levels are split into terms and the terms are split by spin-orbit interactions giving "fine structure". The energy splitting due to fine structure can be written

$$\Delta E_{\text{fs}} = \frac{5.8Z^4}{n^3 l(l+1)}$$

The levels are labelled by quantum numbers (n, l, s, j). The "Z4" factor results in very large "fine structure" splitting for heavy elements (large Z) eg. 107cm−1 in Uranium! This structure was relatively easy to measure and for a long time such measurements gave the most accurate values of _, the fine structure constant. The X-ray lines have a multiplet structure governed by selection rules:

$$\Delta l = \pm 1, \Delta j = 0, \pm 1$$

e.g. the K_a line becomes a doublet K_{a1} , K_{a2}.

X-ray absorption

Absorption spectra in the visible or UV-range of the spectrum consist of a series of discrete lines whose wavelengths coverage to a series limit; the ionization limit. The strength of the lines decreases also towards the ionization limit. For shorter wavelengths than this limit the absorption is spectrally continuous and continues to decrease in strength as the absorbed wavelengths get shorter. The discrete absorption spectrum, the series of discrete lines, is the result of transitions of a valence electron to higher, vacanct, energy levels. Beyond the series limit, absorption results in photoionization; the bound electron is excited to an unbound, free state known as the continuum. The probability of the photoionization decreases with increasing energy of the incident photon because it becomes increasingly difficult for the photon/atom system to conserve both energy and momentum in the interaction. The valence electrons are relatively weakly bound to the massive nucleus and so cannot easily transfer momentum to the nucleus. When the incident photons have X-ray

energies they may raise an inner shell electron to an empty shell (valence shell) or eject it from the atom (photoionization). On the scale of X-ray energies the valence shell energies are negligible so photoionization is the most likely result. Once the threshold energy for photoionizing an inner-shell electron is exceeded there is a sudden increase in the absorption probability. The sharp increase in absorption coefficient associated with such a threshold is called an absorption edge.
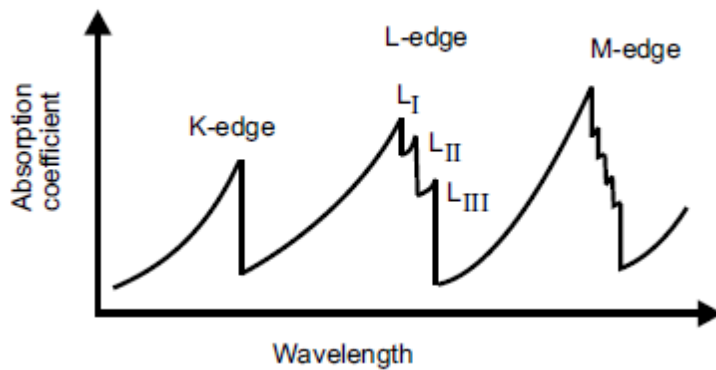

These absorption edges are labelled according to the quantum number of the shell; K edge (n = 1) L edge (n = 2) M, N etc. Each edge exhibits the fine structure of the shells. Thus the M edge (n = 3) has 5 subsidiary edges associated with spin-orbit splitting of the angular momentum states, 2S1/2, 2P1/2,3/2, 2D3/2,5/2. The L-edge has 3 steps and the K-edge is single. When an absorption edge is examined with high spectral resolution it may be found to consist of a few broad peaks that merge into the continuum. These features cover a range of typically 10eV and correspond to transitions from the inner shell to one of the vacancy valence electron shells. These absorption features are broadened by "lifetime broadening" since the Einstein A-coefficient scales with _3, the cube of the transition frequency. (Recall that A=1/_, where _ is the lifetime of the upper state against radiative decay.) As a result of this broadening only a few of these transitions can be resolved. Above an absorption edge, the absorption coefficients drops off until the photon energy exceeds the next inner shell binding energy and a new edge is observed. At the K-edge, for example, the photon energy is capable of ejecting an L or M shell electron. It is more likely, however to eject the K-shell electron which is more strongly bound to the nucleus than any of the higher shell electrons. As a result the excess momentum is more effectively transferred to the nucleus. So those electrons held most

strongly to the nucleus are most effective in absorbing X-ray photons. This effect partly explains the rapid change in absorption at the edge and the fall-off in absorption for energies above each edge.

Auger Effect

The creation of a vacancy in, say, the K-shell is followed by one of two processes.

• Emission of characteristic X-rays as already described.

• The ejection of a second electron and emission of longer wavelength X-rays. This is the Auger effect.
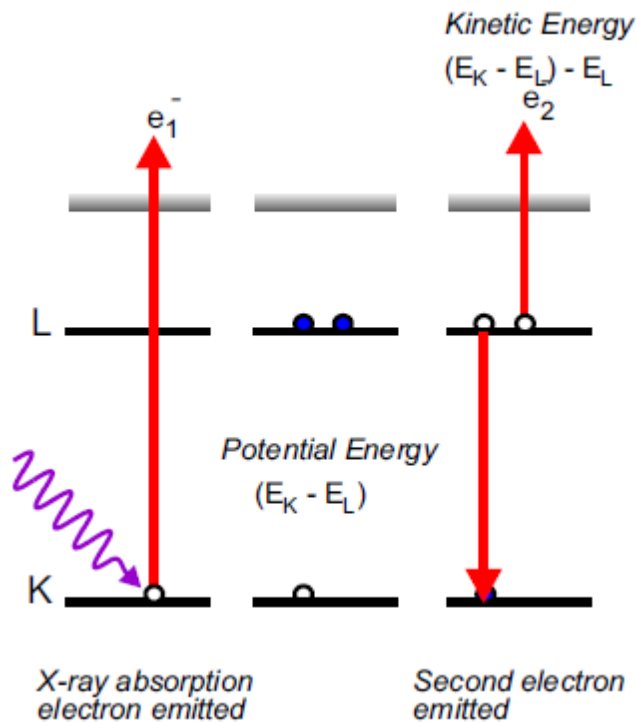
The Auger effect arises because the vacancy in the lower shell (in this case the K-shell creates potential energy that is shared by all the L-shell (and higher shell) electrons. When one L-electron falls in the K-shell vacancy it can give up its energy either as an X-ray (K_a line) or as kinetic energy to another L-shell electron. The donated energy is $E_K - E_L$ and may exceed the L-shell binding energy. If $(E_K - E_L) > E_L$ then this L-shell electron has enough kinetic energy to escape. The resulting ejected electron has kinetic energy $(E_K - E_L) - E_L = E_K - 2E_L$. This Auger effect

is analogous to autoionization from doubly excited states in two electron atoms. There are now two vacancies in the L-shell that can be filled by electrons "falling" from higher shells. This leads to emission of longer wavelength X-rays than the K-series or further Auger processes may occur.

Production of X-rays

An X-ray tube is a vacuum tube designed to produce X-ray photons. The first X-ray tube was invented by Sir William Crookes. The Crookes tube is also called a discharge tube or cold cathode tube. A schematic x-ray tube is shown below.
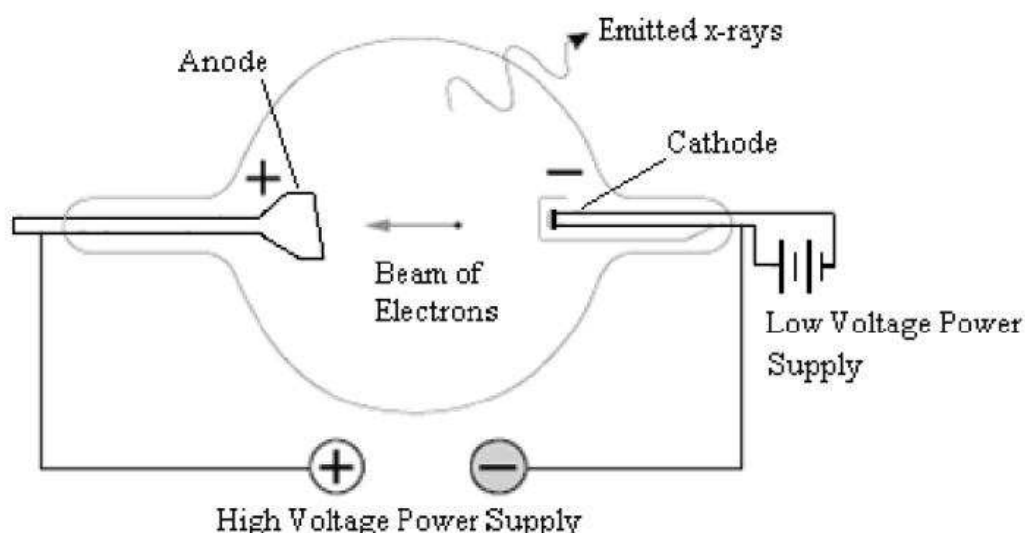
The glass tube is evacuated to a pressure of air, of about 100 pascals, recall that atmospheric pressure is 106 pascals. The anode is a thick metallic target; it is so made in order to quickly dissipate thermal energy that results from bombardment with the cathode rays. A high voltage, between 30 to 150 kV, is applied between the electrodes; this induces an ionization of the residual air, and thus a beam of electrons from the cathode to the anode ensues. When these electrons hit the target, they are slowed down, producing the X-rays. The X-ray photon-generating effect is generally called the Bremsstrahlung effect, a contraction of the German "brems" for braking, and "strahlung" for radiation. The radiation energy from an X-ray tube consists of discrete energies constituting a line spectrum and a continuous spectrum providing the background to the line spectrum.

Properties of X-rays

a- X-rays travel in straight lines.
b- X-rays cannot be deflected by electric field or magnetic field.
c- X-rays have a high penetrating power.
d- Photographic film is blackened by X-rays.
e- Fluorescent materials glow when X-rays are directed at them. Photoelectric emission can be produced by X-rays.
f- Ionization of a gas results when an X-ray beam is passed through it.

X-Ray Diffraction

A plane of atoms in a crystal, also called a Bragg plane, reflects X-ray radiation in exactly the same manner that light is reflected from a plane mirror, as shown in Fig.
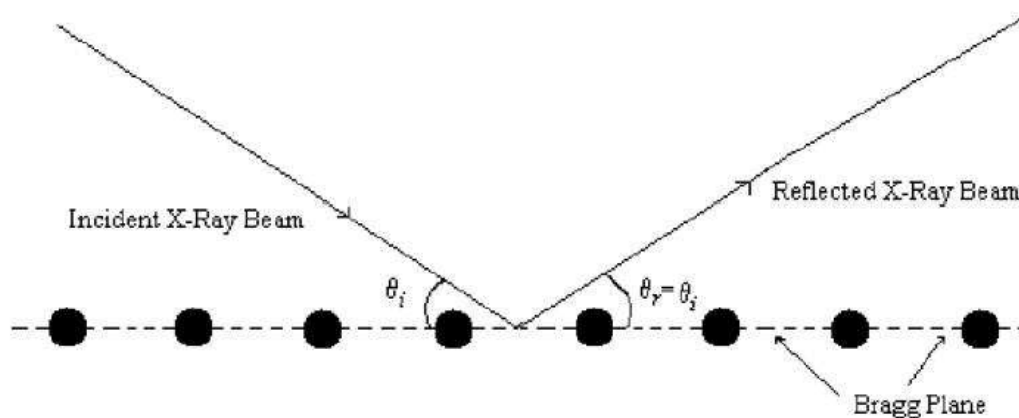
Reflection from successive planes can interfere constructively if the path difference between two rays is equal to an integral number of wavelengths. This statement is called Bragg's law.
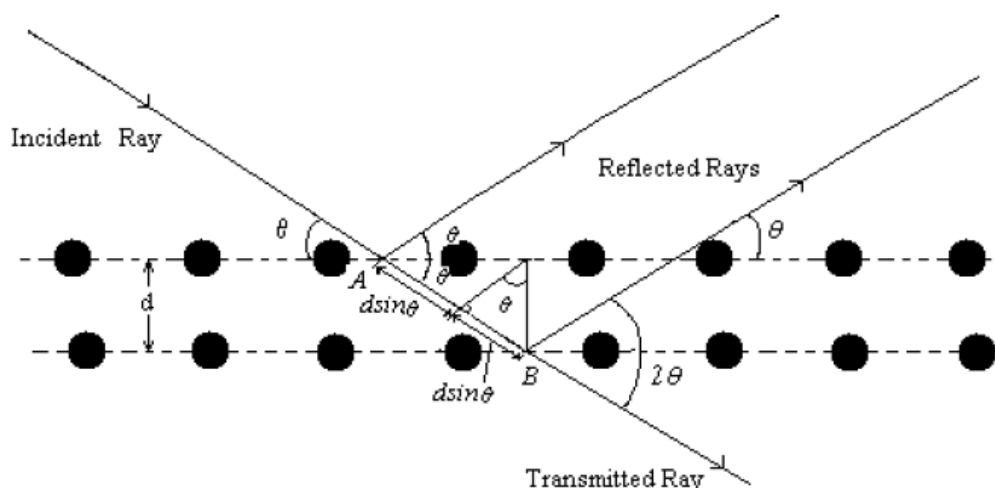
From Fig. above, AB = 2dsinθ so that by Bragg's law, we have 2d sinθ = nλ Where in practice, it is normal to assume first order diffraction so that n = 1. A given set of atomic planes gives rise a reflection at one angle, seen as a spot or a ring in a diffraction pattern also called a diffractogram.

Wave and Particle Theory

What is meant is that the rays behave in some experiments as if they were wave motion and in others as if they were particle motion. The first case depends on the path or paths that the light passes through, as in the interference experiment in which the path difference is calculated. It can be said that light or electromagnetic rays behave as a wave in reflections, refractions, interference, diffraction and polarization.

The second case, the photoelectric phenomenon revealed that the nature of light energy is particles and is emitted by a light source whose frequency is υ, which are photons with separate energies and behave as particles. So to sum up, the photons are of a material nature once and of a wave nature again, that is, according to the conditions to which the photon is exposed.

De Broglie hypothesis

Based on an equation that relates energy and momentum according to the theory of relativity

$$p = \frac{E}{c} = \frac{h\upsilon}{c} = \frac{h}{\lambda}$$

$$\therefore \lambda = \frac{h}{p}$$

So de Broglie assumed that the above equation is a general law that includes photons and material particles, so if light sometimes behaves as a wave and at other times as particles, then particles such as electrons, protons, atoms and molecules must behave in a similar way, that is, they must be accompanied by a certain wave property.

De Broglie assumed the momentum of a body of mass m is p and its velocity v, so that the de Broglie wavelength associated with the particle's motion is

$$\lambda = \frac{h}{mv}$$

Example Calculate the associated wavelength of a 1kg particle moving at 2 x 10^3 m/sec.

$$\lambda = \frac{h}{mv} = \frac{6.625 \times 10^{-34} J.\sec}{1kg \times 2 \times 10^3 m / \sec} = 3.32 \times 10^{-37} m$$

Wave Function ψ

It is a variable quantity that expresses the wave, and that the value of this function depends on the probability of the moving particle being located in place (x,y,z) and at time t, and that the probability of the particle having wave function ψ at the location (x,y,z) and time t is proportional to $|\psi|^2$

In the same space and time, $|\psi|^2$ is the square of the absolute value of the wave function and is called the probability density. When the wave function ψ is a complex quantity that has a real part and an imaginary part, the wave function represents

$$\psi = A + iB \Rightarrow\Rightarrow \psi\psi^* = A^2 - i^2B^2 = A^2 + B^2$$

$$i = \sqrt{-1}$$

De Broglie wave speed

If the object is moving, it will be accompanied by a wave of velocity of this wave

$$\omega = \upsilon\lambda \qquad\qquad \textit{ω wave velocity}$$

This is determined by the velocity of the particle. We note that the velocity of the de Broglie wave is faster than light. This idea does not contradict the theory of relativity, which prevents the speed of the body from reaching the speed of light, because the theory of relativity emphasizes that velocity is responsible for the transfer of mass and energy, while the speed of the accompanying wave is not. On the transfer of mass and energy

$$E = h\upsilon \qquad\qquad \upsilon = \frac{E}{h} = \frac{mc^2}{h}$$

$$\omega = \frac{mc^2}{h} \cdot \frac{h}{mv} = \frac{c^2}{v}$$

In order to understand this result, it is necessary to understand the velocity of the wave and the velocity of the wave group. Let's imagine there is a tight rope on the x axis and its parts oscillate with a simple harmonic movement, at time t = 0 and x = 0 and this is represented before the start of the vibration and we shake the rope, the wave moves with a distance

$$x = \omega t$$

At time t and the interval between x=0 and the point x

$$t = \frac{x}{\omega}$$

We note that the displacement y at point x and time t is equal to the displacement y at point $x = 0$ and the moment $t = \frac{x}{\omega}$ after substitution

$$y = A \cos \omega t \qquad y = A \cos 2\pi \upsilon t$$

$$y = A \cos 2\pi \upsilon (t - \frac{x}{\omega}) = A \cos 2\pi \left(\upsilon t - \frac{\upsilon x}{\omega} \right)$$

$$y = A \cos 2\pi (\upsilon t - \frac{x}{\lambda}) = A \cos \left(2\pi \upsilon t - \frac{2\pi x}{\lambda} \right)$$

$$k = \frac{2\pi}{\lambda}$$

$$y = A \cos (\omega t - kx) = A \cos (\omega t - kr)$$

An equation representing in terms of the three coordinates k is the wave number and r is the radius vector

Uncertainty principle

Heisenberg showed that the position and momentum of the particle cannot be determined simultaneously and precisely. This principle was based on the fact that this quantity is determined precisely and that one is according to the following relationship

$$\Delta x \, \Delta p \geq \hbar \qquad\qquad \hbar = \frac{h}{2\pi}$$

Δx represents the indeterminacy of the particle's position and Δp represents the indeterminacy of the particle's momentum. This equation is known as the product of error Δx times the particle's position and the error Δp of the particle's momentum in a measure of x and p is greater or equal to $\hbar = \dfrac{h}{2\pi}$

$$\Delta y\, \Delta p_{y} \geq \hbar$$

Assume a wave group corresponding to a particle located within the distance Δx

$$\Delta x\, \Delta k = 1 \tag{1}$$

$$\lambda = \frac{h}{p} \qquad\qquad k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h}$$

$$\Delta k = \frac{2\pi \Delta p}{h} \tag{2}$$

Substituting (2) into (1), we get

$$\Delta x\, \Delta p = \hbar = \frac{h}{2\pi}$$

If I want to measure the energy E emitted by an atomic process during a period of time Δt If the energy is emitted in the form of electromagnetic waves, the process of determining the time period will affect the measurement of the wave frequency

$$\Delta \upsilon = \frac{1}{\Delta t} \qquad\qquad \Delta E = h\Delta \upsilon = \frac{h}{\Delta t}$$

$$\Delta E\, \Delta t = h \qquad \Delta E\, \Delta t \geq \hbar$$

Question \ Can the electron be located inside the nucleus? The radius of the nucleus is R = 10^{-14} m, which represents the error in the particle's position.

$$\Delta p = \frac{\hbar}{\Delta x} = \frac{1.054 \times 10^{-34}}{10^{-14}} = 1.1 \times 10^{-20}$$

$$T = pc = 1.1 \times 10^{-20} \times 3 \times 10^{8} = 20 MeV$$

If we assume that the electron is inside the nucleus, knowing that the electron's static energy is (0.511MeV), this means that it cannot exist inside the nucleus. If we assume that the electron

It is inside the atom, knowing that the radius of the atom, according to Bohr's theory of the hydrogen atom, is (R = 5 x 10^{11}m), and this represents the error in the particle's location.

$$\Delta p = \frac{\hbar}{\Delta x} = \frac{1.054 \times 10^{-34}}{5 \times 10^{-11}} = 2.1 \times 10^{-24}$$

$$T = \frac{p^{2}}{2m} = \frac{(2.1 \times 10^{-24})^{2}}{2 \times 9.1 \times 10^{-31}} = 2.4 \times 10^{-18} J = 15ev$$

Schrödinger equation

In order to study the Schrödinger equation, we start with the movement of a particle in one dimension of mass m and velocity v.

$$\psi = A e^{i\omega\left(t - \frac{x}{\omega}\right)} \tag{1}$$

$$\omega = 2\pi\upsilon = \lambda\upsilon$$

$$\psi = A e^{2\pi i\left(\upsilon t - \frac{x}{\lambda}\right)} \tag{2}$$

Equation (2) can be written in terms of momentum and energy

$$E = h\upsilon \qquad \upsilon = \frac{E}{h} = \frac{E}{2\pi\hbar} \qquad \lambda = \frac{h}{p} = \frac{2\pi\hbar}{p}$$

$$\psi = A e^{\frac{-i}{\hbar}(Et - px)}$$

(3)

Differentiating equation (3) partially twice with respect to the x-coordinate and once with respect to time t, we get

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\psi$$

(4)

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar}\psi$$

(5)

By rearranging equations (4) and (5), we get

$$p^2 \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2}$$

(6)

$$E\psi = i\hbar \frac{\partial \psi}{\partial t}$$

(7)

We notice from equations (6) and (7) that it is possible to replace the momentum p^2 with the differential relationship $-\hbar^2 \frac{\partial^2 \psi}{\partial x^2}$ with energy E function of $\hbar \frac{\partial \psi}{\partial t}$

It is known that the total energy E is equal to the sum of kinetic energy and potential energy

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

(8)

And by multiplying equation (8) by ψ

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

(9)

And when we substitute p2ψ and Eψ, we get

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi \tag{10}$$

This equation represents the time-dependent Schrödinger equation

$$\psi = Ae^{\frac{-i}{\hbar}(Et-px)} \qquad\qquad \psi = \psi(x)\phi(t)$$

$$\phi(t) = e^{\frac{-i}{\hbar}(Et)}$$

$$\therefore \psi(x,y,z,t) = \psi(x,y,z)e^{\frac{-i}{\hbar}(Et)} \tag{11}$$

And by putting equation (11) in the time-dependent Schrödinger equation

$$E\psi e^{\frac{-iEt}{\hbar}} = -\frac{\hbar^2}{2m}e^{\frac{-iEt}{\hbar}}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi e^{\frac{-iEt}{\hbar}} \tag{12}$$

And by dividing equation (12) by $e^{\frac{-iEt}{\hbar}}$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \tag{13}$$

This represents the non-time-dependent Schrödinger equation, and by inserting the coordinates (x, y, z), we get

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0$$

The electronic structure of the atom

An introduction

The study of the atomic spectrum has provided a lot of valuable information about the structure and distribution of electrons within an atom. Most of the principles and rules that were used in spectroscopy emerged from experimental research and with the development of quantum mechanics, solid theoretical foundations were laid for them. The atom that emits radiation

$$f = \frac{E_i - E_f}{h} \ \text{…………..(1)}$$

where E_i is the energy of the initial state of the atom and E_f is the energy of the final state of the atom. Also, h is Planck's constant and when we use the wave number instead of the frequency in equation (1) we get

$$\bar{f} = \frac{E_i}{ch} - \frac{E_f}{ch} \ \text{……………………………………………(2)}$$

The above equation shows that the wave number for any line in the spectrum is equal to the difference between two terms, i.e.

$$\bar{f} = T_i - T_f \ \text{…………………………………………..(3)}$$

where each term of T, expressed in wave number, represents an atomic energy state or energy level. The atomic spectrum can be classified into two groups: (1) the optical spectrum, and (2) the X-ray spectrum.

Optical Spectrum Series

The lines of any element were classified in series to facilitate the work of selecting lines belonging to the same series, depending on many types of data, including (a) the physical appearance of the lines, i.e. whether they are (sharp) or scattered (b) the method used to form the spectrum, i.e. whether an electric arc is used Or an electric spark (c) How are the spectral lines affected when an electric or magnetic field is applied to the atoms that

emit them, such as the Zeeman phenomenon that we will discuss later.

In the year 1889, Redberk suggested that the light series known at that time could be arranged in such a way that the wave number of any line of the series equals the difference between two terms, as follows:

$$\bar{f} = \bar{f}_\infty - \frac{RZ^2}{(n+\phi)^2} \quad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots(4)$$

where R is the Rydberg constant, n is an integer, and ϕ is a fraction of less than one and is almost constant for all lines of the series. The series approaches the limit for very large values of n and the limit is the wave number that the series approaches as a limit when n approaches infinity.

Also, Z = 1 for the series of neutral atoms, Z = 2 for ions with a single charge, Z = 3 for ions with a dual charge, and so on, and the similarity between the Rydburke relationship and the Bohr frequency condition is self-evident. In the event that the wavenumber of any line of the spectrum series is equal to the difference between a fixed term and a variable term. The constant term is the wavenumber of the end of the series that represents either the letter $\bar{f}_\infty$ or T_1. The variable term is a wavenumber associated with an atomic state described by a given value of the integer n and the constant ϕ.

Among the most numerous sequences of spectral lines of any element of intensity are the main, acute, diffuse, and fundamental sequences.

The series is represented in terms of the Rydburke relationship by the following equations:

main sequence

$$\bar{f} = P_\infty - \frac{R}{(n+P)^2} \quad (n = 2,3,4,.....$$

<div align="right">Sharp series</div>

$$\bar{f} = S_\infty - \frac{R}{(n+P)^2} \quad (n = 2,3,4,.....$$

diffuseness series

$$\bar{f} = D_\infty - \frac{R}{(n+D)^2} \quad (n = 3,4,5.....$$

<div align="right">Fundamental series</div>

$$\bar{f} = F_\infty - \frac{R}{(n+F)^2} \quad (n = 4,5,6.....$$

Where replace $\bar{f}_\infty$ the symbols P_∞, S_∞, D_∞ and F_∞ as well as replace the constant ϕ in the last term with the letters F, D, S, P in the Rydburke relationship and the values of these constants are different as it was found experimentally that the fixed terms have the following values:

$$P_\infty = \frac{R}{(1+S)^2}$$

$$S_\infty = \frac{R}{(2+P)^2}$$

$$D_\infty = \frac{R}{(2+P)^2}$$

$$F_\infty = \frac{R}{(3+D)^2}$$

It can be seen that each of the acute series has the same purpose as the series, and in most cases a shorthand guide is used to write the equations of the different series. By using the letters that appear in the denominator of the concerned term to represent the term. That is, to write np as an abbreviation

for term $R/(n+p)^2$ and nS for term $R/(n+S)^2$ and nD for term $R/(n+D)^2$ and so on. In terms of this demonstration, the lines of the different series are written as follows:

basic series

$$\bar{f} = 1S - nP$$

Sharp series

$$\bar{f} = 2P - nS$$

Diffuseness series

$$\bar{f} = 2P - nD$$

Fundamental series

$$\bar{f} = 3D - nF$$

According to the boundary values of a number of energy states for all elements by analyzing their spectra, even if the wave number of any line is equal to the difference between two terms, but the opposite is not always true, meaning that not all the differences that may be between the boundary values of an atom represent the spectral lines. To explain the absence of certain lines, it is necessary to use The selection rule, which was previously used for the hydrogen atom, but it is difficult to use this method for complex atoms because we have to solve the Schrödinger equation for a system consisting of three or more

particles, and for this reason, approximation methods were used for most of these problems.

Orbital Angular Momentum

The angular momentum of an electron in its orbit can be represented by a vector L plotted perpendicular to the plane of the orbital. In this regard, the unit angular momentum is used $\hbar = h/2\pi$, which is the unit that Bohr set in his theory of the hydrogen atom.

The orbital angular momentum according to Bohr's theorem is $n\phi\hbar$

The $n\phi$ Represents the azimuthal quantum number. The orbital angular momentum according to Schrödinger's theorem is $\sqrt{l(l+1)}\hbar$

where l is the quantum number of orbital angular momentum bound to l=0,1,2,3…n-1 where n is a fundamental quantum number

In the investigation of atoms that contain more than one electron, we will use the vector l to represent the orbital angular momentum vector for one electron and the vector L for the total angular momentum of all the electrons in the atom. And the numerical values of the vector l according to the vector model of the atom are the value of the quantum number of angular momentum l, so when $l = 2$ we will write with the concept that the value of the angular momentum is $\sqrt{l(l+1)}$ which in this case is equal to $\sqrt{6}\hbar$. The total angular momentum vector L for an atom containing more than one electron is the vector sum of the orbital angular momentum vectors of electrons, so
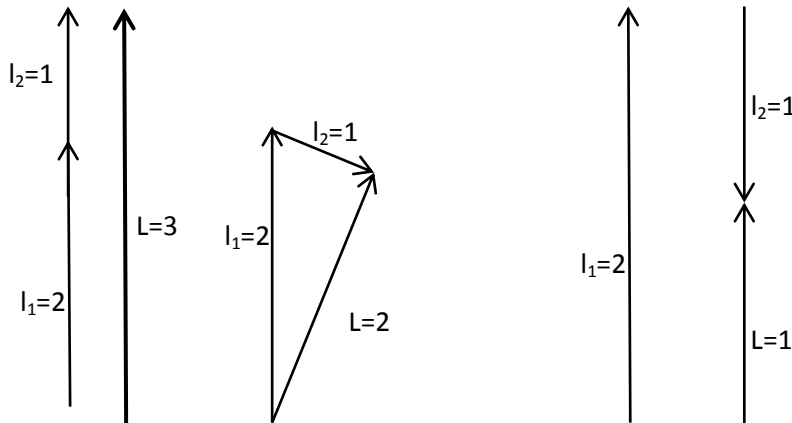
$$\vec{L} = \vec{l}_1 + \vec{l}_2 + \vec{l}_3 + \ldots\ldots$$

With the restriction that the vector is limited to integer values only, for example, in the case of two electrons, one of them is in $l_1 = 2$ and the other is $l_2 = 1$ and the value of the vector

$$\vec{L} = \vec{l}_1 + \vec{l}_2$$

You may take any of the following three values. The figure below shows the method of summing the vectors and the total angular momentum of the two electrons when L = 3

$$\sqrt{L(L+1)}\hbar = \sqrt{12}\hbar$$

The electron's Spin

In addition to the earth's rotation around the sun, there is a throwing motion around its axis. Therefore, the Earth's total angular momentum is the vector sum of its orbital angular momentum and its perpendicular angular momentum. We might expect that the electron also has a spinning motion in addition to its spin motion around the nucleus. But we cannot describe the spin of the electron as a spherical particle because we do not know its exact internal structure. This means that we cannot calculate the angular momentum of an electron in the same way that we calculate the angular momentum of the Earth in terms of its radius and angular velocity.

He proposed the idea of spinning the electron for the first time, Alenic and Kodschmidt, in the year 1926 to explain the exact structure of the lines of the spectral sequences of some elements and the Zeeman phenomenon. The angular momentum of the electron due to spinning is determined by the following value
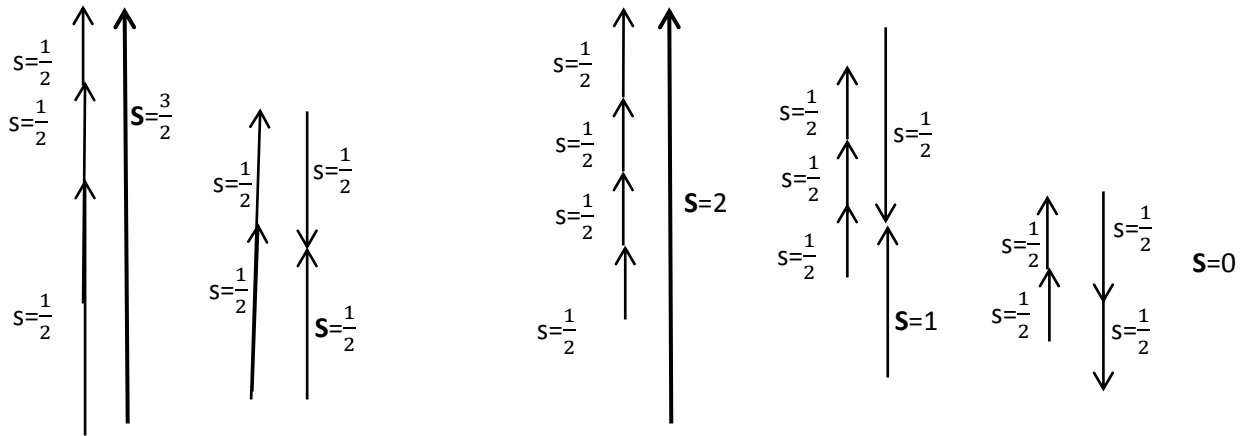
$$\vec{p}_s = s\hbar$$

The magnitude of s is 1/2, and the perpendicular momentum can be represented in terms of algebra of vectors of length s, which is equal to half times ħ. According to quantum mechanics, the magnitude of the spin electron momentum is $\sqrt{s(s+1)}\hbar$ equal, and the vector sum of the spin angle momentum and the number of electrons is subject to the following restrictions

If the number of electrons is odd, then s should take odd multiples of the fraction 1/2

For an even number, s must be an integer, which means that the vectors representing the spin must always be parallel in the same direction or in the opposite direction. The following figure shows two ideal states, one for three electrons in which s takes the values 1/2 or 3/2, and the other for four electrons in which s takes the values 1, 2, 0

It is known that the distribution of electrons in solid materials is subject to the statistical theory developed by Fermi Dirac. One of the features of these distinct particles is that their energy is subject to the Fermi-Dirac statistics and that spinning them equals 1/2 ħ. These particles are called fermions. Such as electrons, protons and neutrons. As for the particles whose spin is equal to the integer numbers of the constant ħ or zero, they are called bosons and they are subject to the statistical theory developed by Einstein and Bose.

$S=\frac{1}{2}$ $S=\frac{1}{2}$ $S=\frac{3}{2}$ $S=\frac{1}{2}$ $S=\frac{1}{2}$ $S=\frac{1}{2}$ $S=\frac{1}{2}$ $S=\frac{1}{2}$

$S=\frac{1}{2}$ $S=\frac{1}{2}$ $S=2$ $S=\frac{1}{2}$ $S=\frac{1}{2}$ $S=\frac{1}{2}$ $S=\frac{1}{2}$ $S=\frac{1}{2}$ $S=\frac{1}{2}$ $S=\frac{1}{2}$ $S=0$

$S=\frac{1}{2}$ $S=1$ $S=\frac{1}{2}$ $S=\frac{1}{2}$

Model Sommerfeld

The Sommerfield atomic model is an extension or addition to the Bohr atomic model. Whereas, in his model, Bohr was able to put equations showing the energy of electrons at each energy level, and he applied this to the hydrogen atom, as well as putting a nice explanation for hydrogen ions, achieving results in agreement with the results of practical experiments, which made his model universally accepted. However, the experiments that took place a few years later using more accurate devices and at higher energies showed that the resulting spectrum was not one line, but rather thin lines that were very close. Bohr could not explain this phenomenon through his atomic model, until Summerfield came to make some modifications to the model to allow the explanation of this phenomenon

According to Sommerfeld, the stationary orbitals in which electrons revolve around the nucleus in an atom are not circular but rather elliptical.

In the picture, the spectrum of the hydrogen atom is on the right and the deuterium atom (an isotope of hydrogen) is on the left
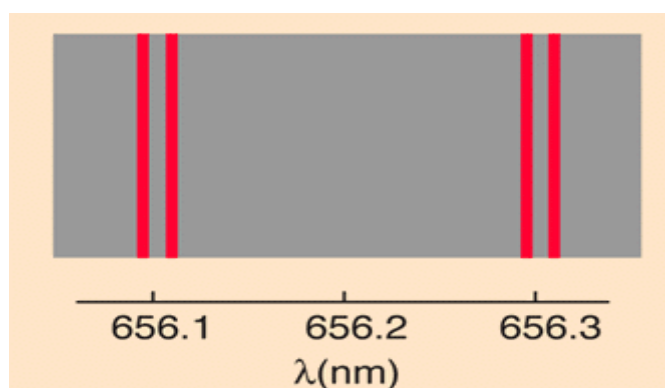
Sommerfield made two major modifications to Bohr's model in order to be able to explain these fine lines:

1- The orbit of the electron around the nucleus is elliptical, with the nucleus at the center of one side.
2- The speed of the electron's movement changes according to its position in the orbit, so that its speed increases as it approaches the nucleus and increases and decreases when it moves away from the nucleus.

Because any oval has two axes, and to determine the ratio between the lengths of the axes, Summerfield used two quantum numbers to determine the shape of the orbit:

1- The original quantum number, which was suggested by Bohr in his theory, which determines the energy of the electron and is symbolized by the letter n

2- The new quantum number, which was called the orbital quantum number and symbolized by the value l, and it determines the value of the angular moment of the electron in its orbit, and this number can take integer values starting with 0 and ending with n-1.

According to Sommerfeld, each level or orbit of electrons has a number of possible sub-paths, i.e. an electron in the n energy level can exist in any sublevel of the sum of n sublevels and one of those sublevels is circular and the rest are in an oval shape.

Using the numbers n and *l*, Summerfield was able to determine the value between the length of the axes of the orbits using the simple equation:

»b/a=(l+1)/n» where a is the length of the longest axis and b is the length of the shorter axis.

Therefore, when n = 1, that is, when the electron is in the first energy level, then the only value of l is 0 and the value of a/b is equal to 1 true, meaning that the shape of the only orbital available is circular.

But when the value of n = 2, we find that the available l values are 0 and 1 and thus we get two values for the ratio of sides length 1 and ½ any circular sub-energy level and another sub-energy level in an oval shape. The electron can exist in any of them according to the value of l and the electron energy varies in If it exists in either of the two sublevels due to the difference in the effective mass of the electron.

In the event that the quantitative number is n = 3, the available values for l are 0.1,2, so that the third level has three paths or sub-levels, one of them is circular, the second is in the ratio of 1/3 sides, and the third is in the ratio of 2/3, as the following figure shows
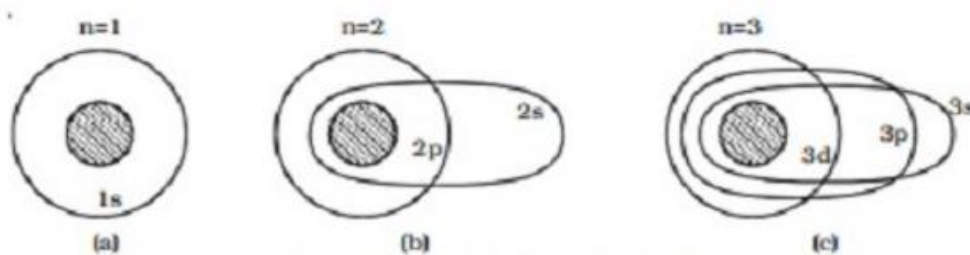
Somerfield symbolized each sub-orbital using the English letters s p d f g when the value of l : 0 1 2 3 4 in order

The sublevel value is expressed by the main level number and then the appropriate letter for the sublevel.

Interpretation of fine lines of the spectrum

Summerfield did not make any modification to Bohr's equations to calculate the energy values of each orbit, as he kept the same variables in the equation, as that equation was relatively accurate and agreed with practical experiments. Also, since no new baseline energy levels are proposed, there are no additional jumps. But since in his special model the paths are elliptical, the effective mass of the electron varies according to its location and speed during its rotation around the nucleus, and thus it became possible to explain the difference in the energy of the thin lines of the spectrum according to the energy of the sub-levels between which the electron moves.

Summerfield then changed the shape of the track from an oval to a rose-like shape.

Somerfield atomic model problems

1- Although the Summerfield model explained the theoretical reason behind the existence of the thin lines that make up the spectrum, it could not accurately predict the number of such lines

2- -The model could not explain the distribution of electrons around the nucleus.

3- Summerfield model could not explain the spectra of alkali metals such as sodium and potassium.

    1- ummerfeld's model could not explain Stark and Zeeman phenomena, which are two phenomena that show that the emitted spectrum may be split and redistributed when exposed to a magnetic field or a very strong electric field.

    2- Summerfield's model could not determine the strength of each thin line of the spectrum.

Zeeman effect

This phenomenon was studied by the scientist Zeeman in the year 1896, where it was observed that the spectral line splits into a group of spectral lines (equal intervals and symmetrical about the original line) as a result of the influence of a constant and regular external magnetic field B. This phenomenon has been called the Normal Zeeman effect, and Lorentz succeeded in explaining this effect using the classical laws of physics, and for this reason the two scientists were awarded the Nobel Prize in Physics in 1902. Classically at the time, this is why it was called the Anomaly Zeeman effect, but with the emergence and development of quantum mechanics theory and the creation of the electron's self-spinning motion, it became easy to explain the anomalous effect of this phenomenon. Despite the success of

quantum mechanics theory in explaining this anomaly, the name is still in use until now.

In the presence of hydrogen-like atoms in the external magnetic field (let's take it in the direction of the Z axis) the total Hamiltonian for the electron takes the form:

$$\hat{H} = \hat{H}_0 + \hat{H}_{LS} + H_B,$$

<div dir="rtl">حيث</div>

$$\hat{H}_0 = -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Ze^2}{r},$$

$$\hat{H}_{LS} = \xi(r)\hat{L}.\hat{S},$$

$$\hat{H}_B = \beta\hat{B}\cdot(\hat{L} + 2\hat{S}) = \beta B(\hat{L}_z + 2\hat{S}_z)$$

m_e is the mass of the electron and β is the Bohr magneton and its value

$$\beta = \frac{e\hbar}{2mc} = 9.27 \times 10^{-24}\,\text{JT}^{-1} = 5.66 \times 10^{-5}\,\text{eVT}^{-1}$$

We will deal here with the characteristic Schrödinger function for atoms similar to the hydrogen atom in spherical coordinates in the image:

$$\Psi \equiv \psi_{nlm}(r,\theta,\varphi)\chi = R_{nl}(r)Y_{l,m_l}(\theta,\varphi)\chi = |n,l,m_l\rangle|s,m_s\rangle$$

We will deal with equation () with the second and third terms as small perturbations, with an important question: which of the terms is greater? Thus, two possibilities will appear to us, which we will talk about in detail:

A - strong magnetic field

For a strong magnetic field, turbulence is dominant, and its strength is sufficient to separate the two influences (meaning that it does not make them couple). Thus, we can deal with their functions in a single way, and the function used is the image, which makes the two effects matrix diagonal. From it we find the correction of the first degree for the outer field gives:

$$\varepsilon_B = \left\langle \hat{H}_B \right\rangle = \left\langle n, l\,', m\,'_l, s\,', m\,'_s \left| \hat{H}_B \right| n, l, m_l, s, m_s \right\rangle$$
$$= \beta B \left(m_l + 2m_s \right)$$

To simplify here and later, all Kroenker delta functions will be neglected $\delta_{m_s, m_s'} \, \delta_{m_l, m_l'} \ldots$

If the electron spin is neglected, the first-order correction gives:

$$\varepsilon_B = \beta B m_l$$

It is said here (as it was previously said about the Stark phenomenon) that the external magnetic field has partially removed the attribute of belonging to the levels (Remove, partially, the degeneracy of the states), or in other words it has separated the levels. We would like to mention that the value of affiliation is defined by the equation (2S+1)(2L+1) for each of the values of L and S.

Example: Study the effect of a strong external magnetic field on the s . plane

We know that the s-level has values $s = \frac{1}{2}, l = 0$, and therefore $m_s = \mp\frac{1}{2}, m_l = 0$ in the presence of the s-level with an external magnetic field, and as a result of the two values $m_s = \mp\frac{1}{2}, m_l = 0$,

the s-level is divided into two levels, and the difference between the energy of the two levels is *2βB*, as in the figure:

			m_l	m_s	ε_B
S			0	1/2	βB
		$2\beta B$			
			0	−1/2	−βB
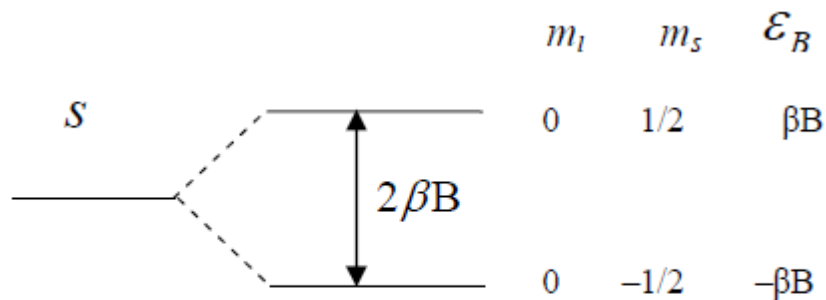
انقسام المدار s في وجود مجال مغناطيسي قوي مع شمول الحركة المغزلية.

Example: Study the effect of an external magnetic field on the p. orbital

The solution We know the electron in the p orbital has the value $l=1$, including $m_l=0, \pm1$ and the value $s=1/2$, including $m_s=\pm1/2$ and from them we make the following table:

:

m_l	$2m_s$	$\varepsilon_B = \beta B(m_l + 2m_s)$
1	1	2
	-1	0
0	1	1
	-1	-1
-1	1	0
	-1	-2

We note that the p orbital was divided into five orbits as a result of the influence of the external magnetic field and the energy takes the values

$$E = E_p \pm 2\beta B \text{,,,,,,} E = E_p \pm \beta B \text{,,,,,,} E = E_p$$

where E_p is the energy of the p orbital before the influence of the external magnetic field. We expected to get six orbitals,

since the multiplicity of these orbitals is calculated from the relationship $(2l+1)(2s+1)=(3)(2)=6$ The orbital with energy $E=E_p$, which is not affected by the field, is derived from the sum of the values $m_l=1$, $m_s=-1/2$ and $m_l=-1$, $m_s=1/2$ and therefore it is a binary orbital as shown in the following figure, which shows the splitting of the p and s orbitals

$\varepsilon_B(\beta B)$ $\qquad\qquad\qquad\qquad$ $\varepsilon_B(\beta B)$

$l=1$ $\quad$ p $\qquad\qquad\qquad$ $+1$ $\qquad\qquad\qquad$ $+2$
$\qquad\qquad\qquad\qquad\qquad$ 0 $\qquad\qquad\qquad$ $+1$
$\qquad\qquad\qquad\qquad\qquad$ -1 $\qquad\qquad\qquad$ 0
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ -1
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ -2

$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $+1$
$l=0$ $\quad$ — $\quad$ S $\qquad\qquad\qquad\qquad$ 0 $\qquad\qquad$ -1
$\qquad\qquad\qquad$ $-1\quad 0\quad 1$

$\qquad\qquad\qquad\qquad\Delta m_l \qquad\qquad m_l$ $\qquad\qquad\qquad m_l+2m_s$

$\qquad B=0$ $\qquad\qquad$ applied magnetic field $\qquad$ applied magnetic field
$\qquad\qquad\qquad\qquad$ excluding the spin $\qquad\qquad$ including the spin