The Fundament of the Mass: The Variant Mass of Electron at Atom

Experimental results: Ionization energy of the electrons at the atom. Bound of the Diatomic Molecules. From Bohr to Schrödinger. Deduction of the radius formula with the analogy of the atom with the blackbody research from Planck and harmonic oscillators. Why the electrons orbit around the nucleus with specific radius for the case of electron as particle. Why the electron doesn't radiate energy at the stationary levels as a wave and as a particle. Diffraction and Interference for the electron by using the Fourier Approach and Wave Properties

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ABSTRACT

Planck wrote in a letter about the research of the energy of the electrons at the cavity of the blackbody: "I knew that the problems of the equilibrium between matter and radiation are of high importance for the Physics. Besides, I knew the right formula for the distribution of the energy spectrum at the cavity. It was very important to find a theoretical interpretation" [9]. After 10 years of research, finally Planck accepted and proposed the quantum theory as explanation to the radiation of the blackbody. The introduction of the Planck constant h was fundamental for the quantization of the energy. The main argument to accept the quantum theory was the concordance with the entropy concept and the statistics thermodynamic. The Einstein research about the quantization of the light radiation at the Photoelectric Effect was also a support for the Planck research of the cavity of the blackbody. Millikan mentioned about the Photoelectric Effect: "The Photoelectric Effect is a proof independent of the quantum theory for the radiation of the blackbody as discrete and discontinuous emission of energy absorbed by the electronic components of the atoms". The Photoelectric Effect supports the constant h discovered by Planck at the research of the blackbody and that the Planck research corresponds to the reality" [9].

Bohr proposed a revolutionary concept for the behavior of the electron during the atom transition from one stationary level to other. In an article research, Bohr mentioned: "The correspondence principle has as consequence the comparison between the atom reaction due a radiation field with the reaction of the atom due a field from the mechanic classic point of view: which is due to a group of virtual harmonic oscillators with frequency equal to the determined for the possible transitions between stationary levels: $h\nu = E - E'$ " [10]. The correspondence principle of Bohr postulated that for high quantum numbers the quantization approach is in correspondence with the classic theory. Therefore, Bohr postulated the quantization of the energy transition for the electrons at the atom ($E - E' = hf$) and the quantization of the angular momentum $L = nh/2\pi$. Bohr could explain the atom stability (the no radiation for the electrons at the atom) with those postulates and obtain a formula for the quantization of the energy, velocity, radius, angular momentum, frequency and wavelength of the radiation emitted or absorbed.

Later, the modern quantum physics could explain the postulates of Bohr and obtain the quantization formula for the energy and angular momentum at the stationary levels by applying the Schrödinger Equation (wave probabilistic theory) and Heisenberg Theory (matrix theory) [4], [5]. The stationary states or levels correspond to those functions which satisfy the Schrödinger Equation [4], [5]. The electron in an atom no excited is at rest. Thus, it cannot radiate energy because it corresponds to a stationary level of the atom [4], [5].

For other hand, Albert Einstein wrote in a research article: "Does the inertia of a body depend on its energy content?" (Ist die Trägheit eines Körpers von seinem Energieinhalt abhängig?) [1]: "If a body emits energy E in the form of radiation, its mass decreases by E/c^2 ". This is true for any type of radiation emitted (gravitational or electromagnetic energy) which produce a decrease in the mass of the body. Thus, Maxwell's theory shows that electromagnetic waves are radiated whenever charges accelerate as for example for the electron. Then, this electromagnetic radiation (photons) produces a decrease in the mass of the electron which is given by the formula of the Variant Mass for an Accelerated Charged Particle which was demonstrated by me at this research [2].

At the atom, the electron only radiates this energy when it jumps from one orbit to another orbit at the atom. It is in accordance with the experimental results from the spectral lines of the atom. The difference is that in a gravitational field the particle or a planet around the sun can take any position at the space and any radius. But, the electron at the atom only can take restricted positions which are explained by quantum mechanics, and the electrons don't emit radiation when they orbit around the nucleus. At this article, it is explained the postulates of Bohr and the reasons for them by using De Broglie approach.

The objective of this research is to demonstrate the discovery formula which describes exactly the variant mass of a charged particle at the atom which emits electromagnetic energy from one stationary level to other. The results of the formula are compared with the ionization energy emission for the electron at the atom and the bound energy for the diatomic molecules. The results are in agreement with high accuracy.

Keywords: Blackbody, Planck Research, Atom Research, Variant Mass, Ionizing Energy Atom, Diatomic Molecules.

1. Introduction

Albert Einstein wrote in a research article entitled: “Does the inertia of a body depend on its energy content? [1]”. Thus, if a particle emits radiation energy E (electromagnetic or gravitational), then the rest energy of the particle decreases in E and by the mass-energy conservation also the mass of the decreases at the same rate E/c^2 [2]. The mass of a body is a measure of its energy content. The inert mass of a body increase or decrease with energy that it contains. If the initial mass of the particle is M and the final mass of the particle is M' , then it is obtained: $M-M'=E/c^2$, $E=(M-M')c^2$, $E=\Delta Mc^2$. The decrease or increase in mass $\Delta M=M-M'$ of the particle is linked to the radiation energy E emitted or absorbed. This energy is also the lost energy of the particle. The radiation carries inertia amid emitting and absorbing bodies [1].

At this research, firstly it is presented the research about the blackbody radiation of Planck, the corpuscular behavior of the radiation (Photoelectric and Compton Effect, Pair Production, Fluorescence, Moseley Plot), the spectral lines of Balmer, the research at the atom of Brown, Rutherford, Bohr, Schrödinger, Heisenberg with the all development of the quantum mechanics, the quantum numbers and atoms with more than one electron. Besides, it is explained why the electron doesn't radiate energy as a particle and a wave and why the electron has restricted radius for the motion at the atom. Also, it is demonstrated the wave-particle duality of De Broglie and the Heisenberg Uncertainty Principle and Diffraction by using the Fourier Approach and Interference Double Slit Experiment by using the wave behavior of the electron. It is also demonstrated the energy levels for the Hydrogen atom by using the Schrödinger Equation. Then, it is showed a research for the bound total energy and energy emission for an electron orbiting the nucleus from a classic point of view. It is demonstrated by theory, calculation and result the discovered formula which describe the mass of an electron which emits electromagnetic energy from one stationary level to other. The formula is in agreement with the bound energy for the particle orbiting the nucleus at the classic limit. Besides, the results of the formula are compared with the ionization energy emission for the electron at the atom and the bound energy for the diatomic molecules. The results between the theoretical formula and the experimental results are in agreement with high precision.

2. Black Body Radiation

2.1. Rayleigh Jeans Formula: Low frequencies

In 1900, Rayleigh and Jeans performed a classical calculation of the energy density of the black body or the cavity heated uniformly to a temperature T valid only for low frequencies. The electrons in the metal walls are thermally agitated and emit electromagnetic radiation within the cavity. In the cavity, a thermal

equilibrium is established and maintained through the absorption and re-radiation of the energy through the walls [9]. Therefore, there are stationary states or waves within each cavity. Rayleigh and Jeans showed that the radiation within each cavity of volume V consists of stationary waves with nodes in the walls [9]. The number of stationary waves for the frequency interval from f to $f + df$ is given by the following formula: $dN = \frac{8\pi V}{c^3} f^2 df$

The classical law of equipartition of energy has established that the average energy is the same for each standing wave in the cavity regardless of its frequency. Thus, the energy is distributed equally for all frequencies. The value of the average energy is given by the formula: $\bar{\epsilon} = kT$ where k is the Boltzmann constant. It only depends on the temperature [9].

The average energy content per unit volume of the cavity for the frequency range from f to $f + df$ is obtained by multiplying the number of standing waves dN by the average energy of the wave kT and dividing it by the volume of the cavity V [9]. The formula obtained is as follows:

$$I(f, T) = \frac{dU}{df} = \frac{8\pi k T f^2}{c^3} \quad \text{Energy density (energy by volume) by frequency unit}$$

$$dU = \frac{8\pi k T f^2}{c^3} df \quad \text{Energy density in the frequency interval } f \text{ to } f+df$$

Fig.1. Black Body and the electromagnetic radiation inside of the cavity where n is the number of stationary waves or nodes. Graph of energy density versus the frequency for the Rayleigh Jeans formula

2.2 Wien Formula: High frequencies

The Rayleigh Jeans formula did not fit the experimental data for high frequencies [5]. The integration over all frequencies for the Rayleigh Jeans formula gives an infinite result for the total intensity of radiation emitted by the body. This was known as the ultraviolet catastrophe.

Fig.2. Graphic of the energy density versus frequency: Wien Formula

Then, Wien proposed a formula with a better fit to these experimental data for high frequencies:

$I(f, T) = \frac{dU}{df} = af^3 e^{-\frac{bf}{kT}}$ Energy density by frequency unit $b=h$: Planck Constant and k is the Boltzmann constant. The values of a and b are obtained by fitting this function with the experimental result.

2.3. Wien Displacement Law for frequency and wavelength

Wien obtained the Wien Displacement Law by using his research for high frequencies. It was obtained by deriving the formula of the energy density and equating it to zero to obtain the value of the frequency where the peak occurs at the energy density graph. This maximum frequency is related with the temperature of the black body:

$f_{\max} = \text{cte } T$ Wien displacement Law

$f_{\max} = 5,879 \cdot 10^{10} T$ constant obtained by experiment results

The Wien law for the wavelength is as follows:

$$dU = af^3 e^{-\frac{bf}{kT}} df \quad dU(T) = I(f, T) df$$

$$c = \lambda f \quad f = c/\lambda \quad df = -c\lambda^{-2} d\lambda$$

$$dU = a \frac{c^4}{\lambda^5} e^{-\frac{bc}{\lambda kT}} d\lambda \quad \text{Energy density for the wavelength interval } \lambda \text{ to } \lambda + d\lambda$$

$$I(\lambda, T) = \frac{dU}{d\lambda} = a \frac{c^4}{\lambda^5} e^{-\frac{bc}{\lambda kT}} \quad \text{Energy density by wavelength unit } b=h$$

The Wien displacement law for the wavelength is as follows:

$\lambda_{\max} T = \text{cte}$ Wien displacement Law

$\lambda_{\max} T = 0,002898$ constant obtained by experiment results.

2.4. Planck Formula

Nevertheless, the Wien formula did not agree with the experimental data for low frequencies. Max Planck solved these difficulties by proposing an empirical formula that could describe all the characteristics of the black body or cavity radiation for all frequencies [5]. Planck postulated the electron oscillators with simple harmonic oscillations and that the energy could take only discrete values:

$$\epsilon_n = n\Delta\epsilon \quad \Delta\epsilon = hf \quad \epsilon_n = nhf$$

$$\epsilon = 0, hf, 2hf, 3hf, \dots \quad n=0, 1, 2, 3, \dots \quad b=h: \text{ Planck constant}$$

It is valid for any physical system that performs simple harmonic oscillations. Later (1905), Einstein assumed in the research of the photoelectric effect that the energy of each mode of oscillation of the

radiation field (light radiation) could also take only certain discrete values, integer multiples of bf , rather than continuous values [9]: $\varepsilon = nbf$ $b=h$. If the energy of the system obeys the Planck quantization $\varepsilon_n = nbf$, the system is quantized, the energy levels are called stationary states or quantum levels and the number n is a main quantum number.

Then, Planck calculated that the average energy $\bar{\varepsilon}$ tends to zero if the $\Delta\varepsilon=bf$ is chosen to be large which corresponds to large frequency, and that it tends to kT if the $\Delta\varepsilon=bf$ is small which corresponds to small frequency [9]. The formula that Planck obtained by interpolation of the two function: Rayleigh and Wien

formula is: $\bar{\varepsilon} = \frac{bf}{e^{kT}-1}$ instead of $\bar{\varepsilon} = kT$ of the Rayleigh Jeans Formula: $du = \frac{8\pi f^2}{c^3} kT df$

Then, it is possible to obtain the Planck formula when using this average energy value instead of kT in the Rayleigh Jeans formula of the energy density in the radiation spectrum of the cavity:

$$du = \frac{8\pi f^2}{c^3} \frac{bf}{e^{kT}-1} df \quad \text{Energy density in the frequency interval } f \text{ to } f+df$$

$$I(f, T) = \frac{du}{df} = \frac{8\pi f^2}{c^3} \frac{bf}{e^{kT}-1} \quad b=h \quad \text{Energy density by frequency unit}$$

Therefore, Planck's great contribution (1901) consisted in proposing that the experimental results could be obtained if the average energy was treated as a discrete variable instead of the continuous variable of classical physics [9].

Fig.3. Graph of the energy density versus frequency for Rayleigh Jeans formula (blue), Wien Formula (turquoise) and the Planck Formula (green)

It is possible to observe at the graphic that the Rayleigh Jeans formula is approximated equal to the Plank formula for low frequencies and the Wien formula is approximated equal to the Planck formula for high frequencies. The constant $b=h$ was determined experimentally and k is the Boltzmann constant. It is known as Planck's constant: $b=h=6,63*10^{-34}$ J s.

The density energy for the wavelength is as follows:

$$du = \frac{8\pi f^2}{c^3} \frac{bf}{e^{kT}-1} df \quad f=c/\lambda \quad df=-(c/\lambda^2) d\lambda \quad b=h: \text{ Planck Constant}$$

$$du = \frac{8\pi}{\lambda^5} \frac{bc}{e^{\lambda kT} - 1} d\lambda$$

$$I(f, T) = \frac{du}{d\lambda} = \frac{8\pi}{\lambda^5} \frac{bc}{e^{\lambda kT} - 1} \quad \text{density energy for the wavelength: Planck Formula}$$

The Planck formula is reduced to the Rayleigh Jeans formula for low frequencies and to the Wien formula for high frequencies [5].

$$I(f, T) = \frac{8\pi f^2}{c^3} \frac{bf}{e^{\frac{bf}{kT}} - 1} \quad e^{\frac{bf}{kT}} = 1 + \frac{bf}{kT} + \left(\frac{bf}{kT}\right)^2 + \dots \quad bf \ll kT \quad (bf/kT)^2 \text{ \& other terms are neglected.}$$

$$I(f, T) = \frac{8\pi kT f^2}{c^3} \quad \text{low frequencies: Rayleigh Jean Formula}$$

It is not necessary to know the value of a and b for low frequencies. For high frequencies, the formula is

$$\text{obtained as follows: } I(f, T) = \frac{8\pi f^2}{c^3} \frac{bf}{e^{\frac{bf}{kT}} - 1}$$

$$I(f, T) = \frac{8\pi f^2}{c^3} \frac{bf}{e^{\frac{bf}{kT}}} \quad e^{(bf/kT)} \gg 1 \quad I(f, T) = \frac{8\pi f^2}{c^3} (bf) e^{-\frac{bf}{kT}}$$

$$I(f, T) = \frac{8\pi b f^3}{c^3} e^{-\frac{bf}{kT}} \quad \text{Wien Formula}$$

$$I(f, T) = a f^3 e^{-\frac{bf}{kT}} \quad a = \frac{8\pi b}{c^3} \quad b = h: \text{ Planck Constant}$$

2.5. Planck Formula from statistics thermodynamic: Boltzmann Distribution

Classical Approach: Continue Energy of the electron oscillators

In the classical calculation of the average energy $\bar{\epsilon}$ of a large number of things of the same kind in mutual equilibrium at temperature T (which leads us to the equipartition law), the average energy is a continuous variable [9]. The equipartition law is a consequence of the Boltzmann distribution which expresses that the probability P(ϵ) that a mode of oscillation has an energy between ϵ and $\epsilon + d\epsilon$ is equal to: $P(\epsilon)d\epsilon =$

$$\frac{e^{-\frac{\epsilon}{kT}}}{Z} d\epsilon \quad Z = \int_0^\infty e^{-\frac{\epsilon}{kT}} d\epsilon \quad Z = kT$$

$$P(\epsilon)d\epsilon = \frac{e^{-\frac{\epsilon}{kT}}}{kT} d\epsilon \quad \bar{\epsilon} = \frac{\int_0^\infty \epsilon P(\epsilon) d\epsilon}{\int_0^\infty P(\epsilon) d\epsilon} = \frac{\int_0^\infty \epsilon \frac{e^{-\frac{\epsilon}{kT}}}{kT} d\epsilon}{\int_0^\infty \frac{e^{-\frac{\epsilon}{kT}}}{kT} d\epsilon} = \frac{\int_0^\infty \epsilon e^{-\frac{\epsilon}{kT}} d\epsilon}{\int_0^\infty e^{-\frac{\epsilon}{kT}} d\epsilon}$$

$$\int_0^\infty \epsilon e^{-\frac{\epsilon}{kT}} d\epsilon = -\epsilon kT e^{-\frac{\epsilon}{kT}} \Big|_0^\infty + kT \int_0^\infty e^{-\frac{\epsilon}{kT}} d\epsilon = (kT)^2$$

$$\bar{\epsilon} = \frac{\int_0^\infty \epsilon e^{-\frac{\epsilon}{kT}} d\epsilon}{\int_0^\infty e^{-\frac{\epsilon}{kT}} d\epsilon} = \frac{(kT)^2}{kT} = kT \quad \text{average continue energy of electron oscillators}$$

$\bar{\epsilon}$ can take any continuous value as the temperature increases. The energy W is given by: $W=N\bar{\epsilon}$ and $W=NkT$ $U=W/V$ where N is the number of stationary waves, U is the energy density and k is the Boltzmann constant. The number of stationary waves for the frequency interval from f to $f + df$ is as follows:

$$dN = \frac{8\pi V}{c^3} f^2 df \quad \frac{dN}{Vdf} = \frac{8\pi f^2}{c^3} \quad \text{density of stationary waves}$$

$$\frac{dU}{df} = \frac{1}{V} \frac{dW}{df} = \frac{1}{V} \frac{dN}{df} kT = \frac{8\pi f^2}{c^3} kT \quad \text{Rayleigh Jeans formula}$$

Quantum Approach: Discrete Energy of the electron oscillators

Planck supposed that the energy could take only certain discrete values given by: $\epsilon=0, \Delta\epsilon, 2\Delta\epsilon, \dots$

$$\epsilon_n = n\Delta\epsilon \quad n=0,1,2,\dots \quad \epsilon: \text{discrete variable}$$

$$\Delta\epsilon=bf \quad \epsilon_n = n\Delta\epsilon = nbf \quad b=h=6.63 \times 10^{-34} \text{J-s} \quad \text{Planck constant}$$

Thus, it is possible to obtain Planck's formula if instead of integrals in the Boltzmann distribution, it is replaced by summations due the discrete energies:

$$\bar{\epsilon} = \frac{\sum_{n=0}^{\infty} \epsilon P(\epsilon) d\epsilon}{\sum_{n=0}^{\infty} P(\epsilon) d\epsilon} \quad \epsilon_n = n\Delta\epsilon = nbf$$

$$P(\epsilon) = \frac{e^{-\frac{\epsilon}{kT}}}{Z} \quad Z = \int_0^{\infty} e^{-\frac{\epsilon}{kT}} d\epsilon \quad Z=kT \quad P(\epsilon) = \frac{e^{-\frac{\epsilon}{kT}}}{kT}$$

$$\bar{\epsilon} = \frac{\sum_{n=0}^{\infty} \epsilon P(\epsilon)}{\sum_{n=0}^{\infty} P(\epsilon)} = \frac{\sum_{n=0}^{\infty} \frac{nbf}{kT} e^{-\frac{nbf}{kT}}}{\sum_{n=0}^{\infty} \frac{e^{-\frac{nbf}{kT}}}{kT}} = \frac{bf \sum_{n=0}^{\infty} n e^{-nx}}{\sum_{n=0}^{\infty} e^{-nx}} \quad \text{where } x = \frac{bf}{kT}$$

$$\bar{\epsilon} = -bf \frac{d}{dx} \ln \sum_{n=0}^{\infty} e^{-nx}$$

$$\sum_{n=0}^{\infty} e^{-nx} = \frac{1}{1-e^{-x}} \quad (\text{Infinite Geometric Progression with } r=e^{-x})$$

$$\bar{\epsilon} = bf \frac{d}{dx} \ln(1 - e^{-x}) = \frac{bf e^{-x}}{(1-e^{-x})} = \frac{bf}{e^x - 1} = \frac{bf}{\frac{bf}{kT} - 1}$$

$$\bar{\epsilon} = \frac{bf}{\frac{bf}{kT} - 1} \quad \text{which is the discrete energy for the electron oscillators.}$$

It is replaced instead of kT at the formula of Rayleigh Jeans: $I(f,T) = \frac{8\pi f^2}{c^3} kT$

$$\text{Then, it is obtained: } I(f,T) = \frac{8\pi f^2}{c^3} \frac{bf}{\frac{bf}{kT} - 1} \quad \text{Planck Formula } b=h$$

$$W=N\bar{\epsilon} \quad W=N \frac{bf}{\frac{bf}{kT} - 1} \quad N: \text{number of stationary waves}$$

$$U=W/V \quad U: \text{energy density}$$

The number of stationary waves for the frequency interval from f to $f + df$ is as follows: $dN = \frac{8\pi V}{c^3} f^2 df$

$$\frac{dN}{Vdf} = \frac{8\pi f^2}{c^3} : \text{density of stationary waves}$$

$$\frac{dU}{df} = \frac{1}{V} \frac{dW}{df} = \frac{1}{V} \frac{dN}{df} \frac{bf}{e^{\frac{bf}{kT}} - 1} = \frac{8\pi f^2}{c^3} \frac{bf}{e^{\frac{bf}{kT}} - 1} \quad \text{Planck formula } b=h$$

This was not necessary to change the Boltzmann distribution. But, it was necessary to postulate that the energy of the oscillators can only take discrete values $\epsilon_n = nhf$ and not continuous values as the classical theory predicts.

2.6. Wien Displacement Formula from Planck Formula

We can obtain the Wien displacement Law: $f_{\max} = cteT$ and $\lambda_{\max} T = cte$ from the Planck formula. It is necessary to obtain the derivative of the density energy by frequency unit formula and equal it to zero:

$$I(f, T) = \frac{8\pi f^2}{c^3} \frac{bf}{e^{\frac{bf}{kT}} - 1} \quad \frac{dI}{df} = \frac{8\pi}{c^3} b \left(\frac{3f^2}{(e^{\frac{bf}{kT}} - 1)} - \frac{f^3 \frac{b}{kT} e^{\frac{bf}{kT}}}{(e^{\frac{bf}{kT}} - 1)^2} \right) = 0$$

$$3(e^{\frac{bf}{kT}} - 1) - \frac{bf}{kT} e^{\frac{bf}{kT}} = 0 \quad x = bf/kT$$

$$3(e^x - 1) - xe^x = 0 \quad (3-x)e^x - 3 = 0$$

It is possible to solve by numerical simulations. It is obtained by applying the Direct Method: $y = (3-x)e^x - 3$

$$x=0 \quad y=0$$

$$x=1 \quad y=2,43$$

$$x=2 \quad y=4,38$$

$$x=3 \quad y=-3$$

Then, the solution must be between 2 and 3. It is possible to do the next table:

x	f(x)	xn-xn-1
2	4,3890561	
2,1	4,34955292	0,1
2,2	4,2200108	0,1
2,3	3,98192772	0,1
2,4	3,61390583	0,1
2,5	3,09124698	0,1
2,6	2,38549521	0,1
2,7	1,46391952	0,1
2,8	0,28892935	0,1
2,81	0,15588446	0,01
2,82	0,01983312	0,01
2,821	0,00606083	0,001
2,8211	0,00468192	0,0001
2,8212	0,0033027	0,0001
2,8213	0,00192318	0,0001
2,8214	0,00054335	0,0001

Table 1. Value of x for the wien displacement formula for frequency

Then, the solution is $x=2,8214$ with a tolerance error of $x_n-x_{n-1}=0,0001$

If we assumed that $b=h$ is known from the Wien Formula by fitting the experimental results, then we can obtain the exact Wien displacement formula:

$$x=bf_{\max}/kT \quad f_{\max} = \frac{xk}{h}T \quad k=1,38065*10^{-23} \text{ J/}^{\circ}\text{K} \quad b=h=6,63*10^{-34} \text{ J s}$$

$$f_{\max}=5,88*10^{10} \text{ T} \quad \text{Wien displacement Law for frequency}$$

If we assumed that the Wien displacement Law is known by the experimental results, then we can obtain the Planck Constant $b=h$:

$$b = \frac{xkT}{f_{\max}} \quad \frac{T}{f_{\max}} = \frac{1}{5,88*10^{10}} \quad k=1,38065*10^{-23} \text{ J/}^{\circ}\text{K} \quad x=2,8214$$

$$b=h=6,63*10^{-34} \text{ J s} \quad \text{Planck Constant}$$

The Wien displacement law for the wavelength is obtained as follows:

$$I(f, T) = \frac{du}{d\lambda} = \frac{8\pi}{\lambda^5} \frac{bc}{e^{\frac{bc}{\lambda kT}} - 1} \quad \text{density energy for the wavelength: Planck Formula}$$

$$\frac{dI}{d\lambda} = 8\pi bc \left(\frac{-5}{\lambda^6 \left(e^{\frac{bc}{\lambda kT}} - 1 \right)} + \frac{\frac{bc}{kT} e^{\frac{bc}{\lambda kT}}}{\lambda^7 \left(e^{\frac{bc}{\lambda kT}} - 1 \right)^2} \right) = 0$$

$$x = \frac{bc}{\lambda kT} \quad -5(e^x - 1) + xe^x = 0 \quad (x - 5)e^x + 5 = 0$$

x	f(x)	xn-xn-1
4	-49,59815	
4,1	-49,3062588	0,1
4,2	-48,3490648	0,1
4,3	-46,5898556	0,1
4,4	-43,8705212	0,1
4,5	-40,0085657	0,1
4,6	-34,7937263	0,1
4,7	-27,9841517	0,1
4,8	-19,3020835	0,1
4,9	-8,42897797	0,1
4,91	-7,2075473	0,01
4,92	-5,96020905	0,01
4,93	-4,68656586	0,01
4,94	-3,38621497	0,01
4,95	-2,0587482	0,01
4,96	-0,70375184	0,01
4,961	-0,56672198	0,001
4,962	-0,42941222	0,001
4,963	-0,29182213	0,001
4,964	-0,15395128	0,001
4,965	-0,01579926	0,001

Table 2. Value of x for the wien displacement formula for wavelength

It is possible to solve by numerical simulations. It is obtained by applying the Direct Method: $y =$

$$(x - 5)e^x + 5$$

$$x=0 \quad y=0$$

$$x=1 \quad y=-5,87$$

$$x=2 \quad y=-17,16$$

$$x=3 \quad y=-35,17$$

$$x=4 \quad y=-49,59$$

$$x=5 \quad y=5$$

Then, the solution must be between 4 and 5. It is possible to do the above table 2:

Then, the solution is $x=4,965$ with a tolerance error of $x_n - x_{n-1} = 0,001$

If we assumed that $b=h$ is known from the Wien Formula by fitting the experimental results, then we can obtain the exact Wien displacement formula:

$$x = \frac{bc}{\lambda_{\max} kT} \quad \lambda_{\max} T = \frac{bc}{kx} \quad \lambda_{\max} T = 0,002898 \quad \text{Wien displacement Law}$$

If we assumed that the Wien displacement Law is known by experiment results, then we can obtain the Planck Constant:

$$b = \frac{kx\lambda_{\max} T}{c} \quad k=1,38065 \cdot 10^{-23} \text{ J/K} \quad x=4,965 \quad c=3 \cdot 10^8 \text{ m/s (light velocity)}$$

$$b=h=6,63 \cdot 10^{-34} \text{ J s} \quad \text{Planck Constant}$$

2.7. Deduction of the Stefan Boltzmann Law $R=\sigma T^4$ and $u = \frac{4}{c} \sigma T^4$

It is considered the radiated energy perpendicular to an area. It should be noted that if the system is in thermal equilibrium, half the energy density of the waves goes towards the walls and half goes out.

$$\frac{dE}{df}: \text{ energy by frequency unit}$$

$$\frac{dR}{df}: \text{ radiation intensity (or power radiation } (\frac{E}{t}) \text{ by area) by frequency unit}$$

$$\frac{dE}{df} = 2 \frac{dR}{df} \Delta t \Delta A \quad \text{formula for a perpendicular radiation energy to the walls.}$$

The number 2 is because the half of the energy goes to the walls and the other half leave from them.

Because, E is the total energy, it is the double of the radiation intensity R .

Fig.4. Energy radiated from a surface

$$\Delta t = \frac{\Delta x}{c} \quad \frac{dE}{df} = 2 \frac{dR}{df} \frac{\Delta x}{c} \Delta A \quad \Delta V = \Delta x \Delta A$$

If the radiation has not the perpendicular direction to the walls, then it is necessary to do some

corrections: $\frac{dE}{df} = 2 \frac{dR}{df \cos \theta} \frac{\Delta V}{\cos \theta c}$

Fig.5. Energy radiated from a Surface with an angle θ

$\Delta R / \cos \theta$ is the component of the power radiation by area in the new direction.

$\Delta x / \cos \theta$ is the component of Δx in the new direction.

$$\frac{dE}{df} = \frac{2}{c} \frac{dR}{df} \frac{\Delta V}{\langle \cos^2 \theta \rangle} \quad \frac{dR}{df} = \frac{c}{2} \frac{du}{df} \langle \cos^2 \theta \rangle \quad du = dE/dV$$

u: energy density given by the Planck Formula

$\langle \cos^2 \theta \rangle$ is the average value for all values of θ from 0 to 2π

$$\langle \cos^2 \theta \rangle = \frac{1}{(2\pi - 0)} \int_0^{2\pi} \cos^2 \theta d\theta = \frac{1}{2\pi} \int_0^{2\pi} \frac{1 + \cos 2\theta}{2} d\theta = \frac{1}{2\pi} (\pi) = \frac{1}{2}$$

$$\frac{dR}{df} = \frac{c}{4} \frac{du}{df} \quad \frac{du}{df} = \frac{8\pi f^2}{c^3} \frac{bf}{e^{kfT} - 1} \quad \text{energy density given by the Planck Formula}$$

$$u = \frac{8\pi b}{c^3} \int_0^\infty \frac{f^3}{e^{kfT} - 1} df \quad x = \frac{bf}{kT} \quad f = \frac{xkT}{b} \quad df = \frac{kT}{b} dx$$

$$u = \frac{8\pi (kT)^4}{(bc)^3} \int_0^\infty \frac{x^3}{e^x - 1} dx \quad u = \frac{8\pi (kT)^4}{(bc)^3} I$$

$$I = \int_0^\infty \frac{x^3}{e^x - 1} dx = \int_0^\infty \frac{x^3 e^{-x}}{1 - e^{-x}} dx = \int_0^\infty x^3 e^{-x} \sum_{k=0}^\infty e^{-kx} dx$$

$$\sum_{k=0}^{\infty} e^{-kx} = 1 + e^{-x} + (e^{-x})^2 + \dots = \frac{1}{1-e^{-x}} \quad \text{Geometric Progression } r=e^{-x}$$

$$I = \int_0^{\infty} \sum_{k=0}^{\infty} x^3 e^{-(k+1)x} dx = \sum_{k=1}^{\infty} \int_0^{\infty} x^3 e^{-kx} dx$$

$$I = \sum_{k=1}^{\infty} \int_0^{\infty} \left(\frac{v}{k}\right)^3 e^{-v} \frac{dv}{k} \quad \text{where } v=kx \quad x=v/k \quad dx=dv/k$$

$$I = \sum_{k=1}^{\infty} \left(\frac{1}{k}\right)^4 \int_0^{\infty} e^{-v} v^3 dv$$

$$\int_0^{\infty} e^{-v} v^{4-1} dv = \Gamma(4) = (4-1)! = 6 \quad \Gamma(n)=(n-1)!: \text{ is the gamma function}$$

$$\sum_{k=1}^{\infty} \left(\frac{1}{k}\right)^4 = \frac{\pi^4}{90}$$

$$I = \frac{\pi^4}{90} (6) = \frac{\pi^4}{15} \quad u = \int_0^{\infty} \frac{du}{df} df = \frac{8\pi(kT)^4}{(bc)^3} I \quad u = \frac{8\pi(kT)^4}{(bc)^3} \frac{\pi^4}{15}$$

$$u = \frac{4}{c} \frac{2\pi^5 k^4}{15b^3 c^2} T^4 \quad \sigma = \frac{2\pi^5 k^4}{15b^3 c^2} \quad \sigma: \text{ Stefan-Boltzmann Constant}$$

$$u = \frac{4}{c} \sigma T^4 \quad u: \text{ energy density: } E/V \quad b=h \text{ Planck Constant}$$

$$\sigma = \frac{2\pi^5 k^4}{15b^3 c^2} \quad \sigma = 5,670 \times 10^{-8} \frac{W}{m^2 \text{ } ^\circ K^4} \quad \text{Stefan-Boltzmann Constant}$$

$$\frac{dR}{df} = \frac{c}{4} \frac{du}{df} \quad R = \frac{c}{4} \int_0^{\infty} \frac{du}{df} df \quad u = \int_0^{\infty} \frac{du}{df} df \quad u = \frac{4}{c} \sigma T^4$$

$$R = \frac{c}{4} u \quad R = \frac{c}{4} \frac{4}{c} \sigma T^4$$

$$R = \sigma T^4 \quad \text{Stefan Boltzmann Law}$$

$$R: \text{ radiation intensity (or power radiation } \left(\frac{E}{t}\right) \text{ by area: } E/(tA))$$

3. Corpuscular behavior of radiation: Photon interaction

Experiments shows that the radiation have wave and corpuscular behavior. Maxwell's equations predict the existence of electromagnetic waves produced by oscillating charges. At the macroscopic world, all the properties exhibited by the radiation (light) are wave behaviors: refraction, reflection, diffraction, polarization and interference (Young Experiment or double slit experiment). Thus, the waves seem to be a perfect way to describe light and other forms of electromagnetic radiation, at least at the macroscopic level [12]. However, at the microscopic level, the electromagnetic radiation exhibits a different set of properties as for example at the Photoelectric effect and Compton effect. The photoelectric effect showed at the microscopic level that light in the nature is granular rather than smooth and that it carries its energy in discrete bundles or packets called photons. Thus, the radiation is composed of photons at the corpuscular theory. Therefore, the interaction between the electromagnetic radiation and the matter at the

microscopic scale, must be described in terms of the interaction between the individual particles (electrons) and the individual photons [12].

The interaction of photons with matter is characterized by the fact that each x ray photon is removed individually from the incident beam in a single event [11]. Thus, the number of photons removed: ΔB is proportional to the thickness traversed Δx (which depends the electron numbers), and to the number of incident photons B : $\Delta B = -\mu B \Delta x$ μ : attenuation coefficient. The absorption occurs where only a certain fraction of the incident radiation (B_0) may pass through the absorber [11]. If this happens, the wavelength of the transmitted beam is unchanged and the transmitted beam B (if the radiation is homogeneous: μ is constant) is described by the next formula (which is the formula for the attenuation of radiation in matter): $B = B_0 e^{-\mu x}$.

A number of photons equal to $B_0 - B$ have been lost in the absorption process, and most of this loss being due to the photoelectric effect. The value of μ referred to the above equation is a function of both the photoelectric absorption (τ) and the scatter (σ) (Rayleigh and Compton Scattering): $\mu = f(\tau) + f(\sigma)$. However, $f(\tau)$ is usually large in comparison with $f(\sigma)$.

Because the photoelectric absorption is made up of absorption in the various atomic levels, it is an atomic number dependent function. A plot of μ/ρ against λ (or energy E) contains a number of discontinuities called absorption edges, at wavelengths corresponding to the binding energies of the electrons in the various subshells [11]. In the energy range being considered from about 50 keV to about 50 MeV for gamma ray photons, most of the interactions are due to: Coherent (Rayleigh) Effect, Photoelectric Effect, Compton Effect, Pair Production [11].

3.1. Coherent (Rayleigh) effect

When a monochromatic X ray beam strikes a target, it may be absorbed (photoelectric effect) or scattered from the atomic nuclei or the electrons. At very low energy of the incident x-ray photon, there is only scattering of the incident photon without energy lost and no ionization. It is known as Rayleigh scattering or Coherent scattering: a X-ray photon collides with one of the electrons of the absorbing element, and the photon is deflected (scattering by the atomic electrons) from its original direction without energy lost (elastic collision) [11], [12].

Rayleigh scattering can be explained by means of the wave theory: it occurs when an electromagnetic wave moves near an electron and excites it into oscillations with the same frequency and with the same phase as the incident photon. Since there is not energy change involved at the process, the coherent scattered radiation will retain exactly the same wavelength as the incident beam. The probability of this effect is proportional to $Z^{2.6}/E^2$ [12].

3.2. Photoelectric Effect (*Quantization of the radiation: light*)

It occurs for low energy photons $E < 200 \text{ keV}$. It can be explained at the wave theory by the next form: the electromagnetic radiation incident on the surface which consists of electric and magnetic fields can exert forces (mainly the electric field) on the electrons of the surface and they can be emitted [5], [11].

Also, it can be also explained at the microscopic level by means of the electromagnetic radiations as composed of photons. An incident photon with sufficient energy is completely absorbed by a bound electron of an atom in the absorber material, and the electrons are ejected (photoelectron). The photon gives all its energy to the bound electron (recoil electron) of the atom at this effect. A bound electron is required to conserve energy and momentum. The electron uses part of the energy to overcome its binding to the atom and takes the rest as kinetic energy. The vacancy left in the atomic structure by the ejected electron is filled by one of the electrons from a higher shell or by a free electron from outside the atom. This transition is accompanied by the emission of a characteristic x-ray. Also, this x ray can be imparted to another electron, which is emitted and it is called Auger electron. The subject of this study is called Fluorescence. The probability of this effect is dependent upon Z , and an approximate expression for the absorption probability τ is: $\frac{Z^n}{E^{3.5}}$ where n is normally between 4 and 5 depending of the absorber material [11].

It was observed at the Photoelectric effect that if the frequency of the incident radiation is very low, then there is no electron ejected. The classic electrodynamic has established that the electrons must be emitted in any frequency if the intensity is enough. The quantization of the electromagnetic radiation solved the contradiction from classic electrodynamic for this experiment [5]. Einstein proposed a corpuscular theory for the incident radiation (light) at the Photoelectric Effect [5]. The formula of the Photoelectric effect is as follows: $hf = K_{\max} + U_0$. U_0 : bound energy of the electron, hf : electron energy.

The bound energy was called work function. It is equal to the minimum energy $E = hf_{\min}$ necessary to eject an electron with kinetic energy almost with zero value: $hf_{\min} = U_0$ $f_{\min} = U_0/h$ $U_0 = \text{work function}$ $K=0$ for $f_{\min}$

If $f < U_0/h$ (very low frequency, very low energy), then there is no electron ejected independent of the radiation intensity. If the frequency is increased: $f \geq U_0/h$ until the value where the energy of a single photon $E = hf$ is more than the bound energy of the electron or work function U_0 : $hf \geq U_0$, then the electron is ejected. The rest of the energy is given to the electron as kinetic energy. Thus, the electron has absorbed the energy of a single photon (with energy $E = hf$) from the electromagnetic radiation [4], [5]. If the radiation intensity (with minimum frequency $f > U_0/h$) increases, then more electrons can be ejected. The maximum kinetic energy of the electron increases linearly with the frequency: $K_{\max} = hf - U_0$. It also

depends on the energy of the incident radiation which at the microscopic level is composed of quantum packets whose energy depends of the frequency ($E=hf$). It is concluded that for a fixed value of frequency, the maximum kinetic energy of the electron always is the same independent of the radiation intensity. Nevertheless, the number of electrons emitted increases with the intensity. Besides, some electrons can be ejected with a kinetic energy less than the $K_{\max}$ because some electrons can lose energy in the collision process at the atom [4], [5].

Planck proposed a quantization of the energy for the electron virtual oscillators in the cavity walls of the blackbody wave theory. Einstein proposed a corpuscular theory for the incident radiation (light) [5]. This photoelectric effect was a proof of the analogy of the atom with the Blackbody Research of Planck: the electrons at the cavity of the blackbody behave as virtual oscillators which absorb and emit energy in discrete packets of energy or photons. At the Photoelectric Effect, the energy of the incident radiation is quantized as discrete quantum energy called also photons.

In resume, this effect was a proof that the energy of the incident radiation (electromagnetic radiation) is composed of packed of energy called photons with energy $E=hf$ which is given to the bound electron. It was also a proof of stationary levels of energy at the atom and the quantization at the Blackbody research from Planck. Therefore, at the microscopic level, there is emission or absorption of energy as discrete packets of energy called photons where the incident energy radiation is the sum of all discrete packets of energy.

In 1916, Millikan conducted a series of experiments that confirmed Einstein's theory of the photoelectric effect. This experiment demonstrated the quantization of the light radiation and the corpuscular theory of Einstein [5]. It was also possible to determine Planck's constant with this experiment [5].

Fig.6. Graphic of the maximum kinetic energy of the photoelectrons versus the frequency of the light for the Photoelectric Effect

The figure shows a linear relationship between the maximum kinetic energy and the frequency: $K_{\max}=hf-U_0$. The constant of Planck was possible to obtain from the slope of the graphic of the maximum electrical potential to stop the electron flux versus the frequency:

$$hf=K_{\max}+U_0 \quad K_{\max}=(1/2)mv^2=eV_{\max}$$

$V_{\max}$: electrical potential necessary to stop the electron flux: retardation potential.

$$hf = eV_{\max} + U_o \quad V_{\max} = (h/e)f - (U_o/e)$$

$$s = h/e \quad (s: \text{slope})$$

$h = s e$ where s is the slope and e is the electric charge of the electron

This same constant that is used for the quantization of the virtual electron oscillators in the black body cavity is used to quantize electromagnetic radiation in the Photoelectric Effect. This constant is called the Planck's constant [5].

It is also possible to determine U_o when $V_{\max} = 0$: $U_o = hf_{\min}$

3.3. Compton Effect

The Compton Effect (incoherent scattering) occurs at energies much greater than the binding energies of the electrons. It is the dominant mode of interaction around 1 MeV (intermediate energy range). As the electromagnetic radiation is composed of photons, the interaction of the electromagnetic radiation with the matter can be described in terms of collisions between the individual particles (electrons) and the individual photons. At this effect, the incident γ photon scatters from an outer shell electron of the atom in the absorber material at an angle Φ . The photons are scattered as if the electrons were free and at rest (loosely bound). The photon gives up a small part of its energy to the loosely bound electron as kinetic energy during the collision. As result of it, the wavelength of the incoherent scattered photon will be greater than λ_o (less energy, less frequency, more wavelength). The photon never lost the whole energy in any one of the collisions. The scattered photons can then continue through the absorber and interact again or scatter out of the absorber material completely. [11], [12]. Typically, the photon will have sufficient energy to produce several recoil electrons. Therefore, all possible energy losses will occur in a x-ray beam. The net result is the production of ion cascades as fast electrons react with other atoms.

The probability of this effect decreases rapidly with the increasing energy and it is also dependent on the number of electrons available Z for the scattering of the photon. The probability of this effect is proportional to Z/E [11],[12]. If the full energy of the incident photon is not absorbed in the detector, then there is a continuous background in the energy spectrum, known as the Compton continuum. This continuum extends up to an energy corresponding to the maximum energy transfer, where there is a sharp cut-off point, known as the Compton Edge (for $\Phi = 180^\circ$: backscattering of the photon). There is a probability that each event has approximately equal chance to produce a pulse with any height up to this maximum. Thus, Compton events will provide a well distributed low-energy area in the spectrum [11], [12]. Arthur Compton performed his experiment in 1923 and at this time it had already been known that

a material illuminated by x-rays gave off what were called secondary rays. The objective of the Compton experiment was to show that these secondary rays were primarily the result of scattering of the incident x-rays from electrons in the material [12].

X-rays of known wavelength were produced in an x-ray tube and allowed to strike a graphite target. A series of slits allowed to enter to the spectrometer to only those scattered x-rays which left the target in a direction making an angle Φ with the direction of the beam of incident x-rays. This angle Φ was the angle through which these particular x-rays had been scattered and its value could be varied by moving the x-ray source [12]. The x-ray spectrometer consisted of a crystal from which the x-rays were reflected and directed to an ionization chamber where the x rays were detected. The wavelength of the scattered x-rays could be determined from the angle at which they were reflected from the crystal with maximum intensity [12].

The scattering of x-rays from free electrons was explainable in terms of the classical electromagnetic wave theory of radiation. The details was worked out by Thomson. Besides, J.A. Gray noticed that the scattered x-rays had the same polarization and roughly the same intensity as were predicted by Thomson's scattering theory, but that the scattered rays were absorbed more readily (less energy) than the incident x-rays. It was verified by Compton and it occurred to him, that this increased absorbability could be explained if one assumed that the wavelength of the scattered x-ray was slightly higher (more wavelength, less energy, less frequency) than the original wavelength of the incident x-rays [12].

The measurements done by Compton of the absorbability of the scattered x-rays over a wide range of incident wavelengths, indicated that the increase in the wavelength of the scattered x-rays was consistent in the order of 0.03A. Then, Compton decided to check this increase wavelength directly, using an x-ray spectrometer [12]. Besides, he checked if the wavelength shift was depended upon the angle Φ through which the x-rays were scattered.

The incident x-rays on the graphite target had a wavelength of $\lambda=0.707$ A. When $\Phi=0^\circ$, the detected x-rays in the spectrometer are essentially those which have undergone with no scattering. Thus, the spectrometer's output is a single peak centered around $\lambda=\lambda'=0.707$ A at this angle [12]. As the value of Φ is increased, the single peak splits up into two peaks, one at the original value of $\lambda=0.707$ A, and the other at the increased wavelength λ' whose value depends upon the value of Φ . Compton showed that at least some of the scattered x-rays had their wavelengths changed in the scattering process. The amount by which the wavelength of a scattered x-ray changed was directly related to the angle Φ through which it had been scattered. The empirical relationship (experimental results) for the shifted peak position was given by: $\Delta\lambda=\lambda'-\lambda=\lambda_c(1-\cos\Phi)$ where λ' : scattered x-rays wavelength, λ : incident x-rays wavelength, $\lambda_c=h/(m_e c)=0,0243$ A: electron Compton wavelength, and Φ : scattered angle of x-rays [12].

The photons carries a specific amount of momentum and energy and they behaves like particles with a rest mass of zero. The standard rules of relativistic kinematics apply to these collisions, and it can be used to determine the properties of the scattered radiation [12].

Fig.7. The Compton interaction

Momentum Conservation

$p_\gamma = p_\gamma' \cos \Phi + p_e' \cos \theta$ $p_e = 0$ because initially the electron is at rest.

$$0 = p_\gamma' \sin \Phi - p_e' \sin \theta$$

$$p_\gamma - p_\gamma' \cos \Phi = p_e' \cos \theta$$

$$p_\gamma' \sin \Phi = p_e' \sin \theta$$

By squaring both sides of the two equations and adding both equations, it is obtained:

$$p_\gamma^2 - 2 p_\gamma p_\gamma' \cos \Phi + p_\gamma'^2 = p_e'^2$$

Energy Conservation

$$m_e c^2 + E_\gamma = E_e' + E_\gamma' \quad m_e = m_0 : \text{rest mass of the electron} \quad p_e = 0$$

$$E_e' = m_e c^2 + E_\gamma - E_\gamma' \quad K = E_\gamma - E_\gamma'$$

$$E_e' = m_e c^2 + K \quad \text{Total Energy for the electron}$$

By using the Dirac equation and the total energy for the electron, it is obtained:

$$E_e'^2 = p_e'^2 c^2 + m_e^2 c^4 \quad \text{Dirac Equation}$$

$$E_e' = m_e c^2 + K \quad \text{Total Energy for the electron}$$

$$(m_e c^2 + K)^2 = p_e'^2 c^2 + m_e^2 c^4$$

$$m_e^2 c^4 + 2 m_e c^2 K + K^2 = p_e'^2 c^2 + m_e^2 c^4$$

$$2 m_e c^2 K + K^2 = p_e'^2 c^2$$

$$2 m_e K + \frac{K^2}{c^2} = p_e'^2$$

$$p_{\gamma}^2 - 2 p_{\gamma} p_{\gamma'} \cos\Phi + p_{\gamma'}^2 = p_e^2$$

$$2 m_e K + \frac{K^2}{c^2} = p_{\gamma}^2 - 2 p_{\gamma} p_{\gamma'} \cos\Phi + p_{\gamma'}^2$$

$$p_{\gamma} = h/\lambda \quad p_{\gamma'} = h/\lambda' \quad K = E_{\gamma} - E_{\gamma'} \quad K = (hc/\lambda) - (hc/\lambda')$$

$$2 m_e \left(\frac{hc}{\lambda} - \frac{hc}{\lambda'} \right) + \frac{\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'} \right)^2}{c^2} = \left(\frac{h}{\lambda} \right)^2 - 2 \left(\frac{h}{\lambda} \right) \left(\frac{h}{\lambda'} \right) \cos\Phi + \left(\frac{h}{\lambda'} \right)^2$$

$$2 m_e hc \left(\frac{1}{\lambda} - \frac{1}{\lambda'} \right) + \left(\frac{h}{\lambda} \right)^2 - 2 \left(\frac{h}{\lambda} \right) \left(\frac{h}{\lambda'} \right) \cos\Phi + \left(\frac{h}{\lambda'} \right)^2 = \left(\frac{h}{\lambda} \right)^2 - 2 \left(\frac{h}{\lambda} \right) \left(\frac{h}{\lambda'} \right) \cos\Phi + \left(\frac{h}{\lambda'} \right)^2$$

$$2 m_e hc \left(\frac{1}{\lambda} - \frac{1}{\lambda'} \right) = 2 \left(\frac{h}{\lambda} \right) \left(\frac{h}{\lambda'} \right) (1 - \cos\Phi)$$

$$m_e c \left(\frac{\lambda' - \lambda}{\lambda \lambda'} \right) = \frac{h}{\lambda \lambda'} (1 - \cos\Phi)$$

$$\lambda' - \lambda = \Delta\lambda = \frac{h}{m_e c} (1 - \cos\Phi) \quad \textbf{Compton wavelength formula} \quad m_e = m_0$$

λ : wavelength of incident radiation λ' : wavelength of scattered radiation

where $\lambda_c = \frac{h}{m_e c}$ is the Compton wavelength $\lambda_c = 0,0243 \cdot 10^{-10} \text{ m}$

$$\frac{hc}{E'} - \frac{hc}{E} = \frac{h}{m_e c} (1 - \cos\Phi) \quad E = hf = hc/\lambda \quad \lambda = hc/E$$

$$E'_{\gamma} = \frac{E_{\gamma}}{1 + \frac{E_{\gamma}}{m_e c^2} (1 - \cos\Phi)} \quad \textbf{Energy of the scattered photon} \quad m_e = m_0$$

Where, E_{γ} is the incident photon energy, E_{γ}' is the energy of the scattered photon.

The kinetic energy of the electron after the collision is given by:

$$K = E_{\gamma} - E'_{\gamma} = E_{\gamma} - \frac{E_{\gamma}}{1 + \frac{E_{\gamma}}{m_e c^2} (1 - \cos\Phi)}$$

$$K = E_{\gamma} - E'_{\gamma} = \frac{E_{\gamma}^2 (1 - \cos\Phi)}{m_e c^2 + E_{\gamma} (1 - \cos\Phi)} \quad m_e = m_0$$

$$\text{where: } E_e' = m_e c^2 + K \quad E_e' = m_e c^2 + hf - hf' \quad K = hf - hf' \quad m_e = m_0.$$

It can be seen that since all scattering angles for the photons are possible, the electron energy ranges from $K=0$ for $\Phi=0^\circ$ to $K=2E_{\gamma}^2/(m_e c^2 + 2E_{\gamma})$ for $\Phi=180^\circ$ (maximum energy which can be transferred to the electron). It was assumed in the derivation of the Compton wavelength shift equation, that the electron involved was free, rather than being bound to an atom. If the electron had been bound to the atom, the situation would have been quite different, since also the atom would have been involved in the collision. The assumption is valid for electrons lightly bound with energies of few eV and for photon energies

much bigger than it, in the order of keV or more [12].

3.4. Pair Production

Pair production occurs with high energy γ rays of energy in the range of 5-10 MeV. It is produced by high energy cosmic gamma rays (photons) or high energy gamma rays emitted by radioactive substances or in laboratory due bremsstrahlung photons produced in particle accelerators. It is the process in which a high energy photon in the field of a nucleus or an electron disappears with the creation of an electron-positron pair. The positrons (positive charge) are the antiparticle of the electron (negative charge). It has similar properties of the electron but the charge and the magnetic momentum is opposite to the electron.

Fig.8. Pair Production

The nucleus goes back in opposite direction to the direction of the electron-positron motion. The nucleus energy is very small and neglected due the high value of the nucleus mass (very low recoil velocity). Nevertheless, the presence of the nucleus is necessary for the momentum conservation. The total kinetic energy of the resultant particles is equal to the photon energy minus the rest mass energy of the two particles which have been created. The equation that express this relation is as follows: $hf = E_e + E_p$

$$E_e = m_e c^2 + K_e \quad E_p = m_p c^2 + K_p \quad m_p = m_e$$

$$hf = 2m_e c^2 + K_e + K_p$$

The minimum energy $E = hf_{\min}$ to create the electron-positron pair is given by the next formula:

$$E = hf_{\min} = 2m_e c^2 \quad K=0$$

$$E = hf_{\min} = 1.022 \text{ MeV} \quad f_{\min} = 2,4 \cdot 10^{20} \text{ Hz} \quad f = c/\lambda \quad \lambda_{\max} = 0.012 \text{ A}$$

Thus, if the photon energy is greater than $1.022 \text{ MeV} = 2m_e c^2$ ($E > 1.022 \text{ MeV}$, $f > 1.022/h$ $f > 2,4 \cdot 10^{20} \text{ Hz}$ or $\lambda < hc/1.022$ $\lambda < 0.012 \text{ A}$) in presence of an atomic nucleus, then an electron positron pair is created and the residual energy is distributed evenly between the electron and positron as kinetic energy. After, the positron is combined with one electron in a bound system called positronium. The electron and the positron moves around of the mass center of this system. Then, the positron is annihilated with the atomic electron producing two γ rays (photons) of energy 511 keV. The half life of the positron is very short (10^{-10} s) [11]. The total charge is conserved at this process and the kinetic energy of the positron is a little

more than the kinetic energy of the electron. It is because the positive charge of the nucleus accelerates to the positron and dis-accelerates to the electron. The cross section for this process shows that it varies with Z approximately as Z^2 . For higher Z materials, this dominance will occur at a lower energy.

3.5. Pair Annihilation

It is the opposite process to the pair creation. An electron and positron (particle and antiparticle) initially at rest and close between them are attracted and annihilated. At this process, the matter disappears and it is converted in energy radiation or photons. It is no possible to create only one photon because the momentum needs to be conserved. It is possible to create two photons or more but the two photons creation is the process more probable. The two photons are created with equal momentum but with opposite sign. Then, they moves each from the other in opposite direction. Each photon has equal energy of 511 keV. The momentum conservation requires that the momentum of the two photon needs to be equal: $0=p_1-p_2$ $p_1=p_2$ $p=hf$ $f_1=f_2=f$ $c=\lambda f$ $\lambda_1=\lambda_2=\lambda$

The energy of each photon is equal to $E=hf$

$$hf=m_e c^2=0.511 \text{ MeV}$$

$$hc/\lambda=m_e c^2$$

$$\lambda = \frac{h}{m_e c} \text{ which is equal to the Compton wavelength } \lambda=0,0243 \text{ A}$$

3.6. Fluorescence, Moseley Plot

X-rays can be described in 2 ways: electromagnetic wave or particle (photon). In the electromagnetic spectrum, we can see that the photon energies of the x-rays are between 100 eV and 100 keV, the wavelength between 10^{-8} and 10^{-12} m, and the frequency between 10^{16} and 10^{20} Hz.

X-ray fluorescence (XRF) is the phenomenon where a material is exposed to X-rays of high energy, and as the X-ray (or photon) strikes an atom (or a molecule) in the sample, the energy is absorbed by the electron at the atom. If the energy is high enough, a core electron is ejected out of its atomic orbital (lifted into the continuum) as the Photoelectric Effect has established. Then, an electron from an outer shell drops into the unoccupied orbit or level to fill the hole left behind. This transition gives off a X-ray photon of fixed characteristic energy (Fluorescence X-ray) that can be detected by a fluorescence detector. The energy needed to eject a core electron is characteristic of each element. Besides, the energy emitted by the transition is also characteristic of each element. Thus, it is possible to discover the material which is composed a sample by using Fluorescence X-rays [11]. X-rays were first discovered by Wilhelm K. Roentgen in 1895. In 1913, Henry Moseley, measured and plotted the x-ray frequencies for about 40 of the elements of the periodic table. He showed that the K-alpha x-rays followed a straight line

when the atomic number Z versus the square root of frequency was plotted [11]. With the insights from the Bohr model, we can write his empirical relationship as follows: $\Delta E = hf = hcRZ^2\left(\frac{1}{n'^2} - \frac{1}{n^2}\right)$

energy spectral lines

$$\Delta E = hcR(Z - 1)^2 \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad R = \frac{me^4}{8\epsilon_0^2 cb^3} : \text{Rydberg Constant}$$

$$\Delta E = hf = 13.6 \text{ eV} (Z - 1)^2 \left(\frac{1}{1^2} - \frac{1}{2^2} \right) = \frac{3}{4} 13.6 \text{ eV} (Z - 1)^2$$

$$(Z - \sigma) = (Z - 1) \quad \sigma = 1: \text{shielding constant } \sigma \leq 1 \quad n' = 1 \quad n = 2 \text{ K}\alpha \text{ lines}$$

$$Z = \sqrt{\frac{4h}{(3)(13.6)}} \sqrt{f} + 1 \quad Z = 2,016 * 10^{-8} \sqrt{f} + 1 \quad Z \text{ versus } \sqrt{f}: \text{ Moseley Plot}$$

Fig.9. Moseley's plot: atomic number Z vs square root of frequency $\sqrt{f} * 10^{-8}$ (f in Hz) for the K_α lines

It is also possible to obtain the relationship between the wavelength of a characteristic X-ray photon and the atomic number Z of the excited element:

$$\frac{1}{\lambda} = R(Z - \sigma)^2 \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad R: \text{Rydberg Constant} \quad R = \frac{me^4}{8\epsilon_0^2 cb^3}$$

The reciprocal of the square root of the wavelength as a function of atomic number, for the K, L and M series (which can be graphed) is obtained as follows:

$$\frac{1}{\sqrt{\lambda}} = \sqrt{R \frac{3}{4}} (Z - 1) \quad \delta = 3R/4 \quad \sigma = 1 \text{ shielding constant } \sigma \leq 1 \quad n' = 1 \quad n = 2 \quad K\alpha \text{ lines}$$

δ is a constant that takes different values for each spectral series

The primary source unit of x-rays consists of a very stable high-voltage generator, capable of providing a potential of typically 40–100 kV. The current from the generator is fed to the filament of the X-ray tube. X-rays are produced when the electrons are suddenly decelerated with a high voltage (accelerated charges give off electromagnetic radiation from the Maxwell Theory), upon the collision with the metal target (as tungsten for example). These x-rays are commonly called bremsstrahlung or "braking radiation" (white radiation also). If the bombarding electrons have sufficient energy, they can knock an

electron out of an inner shell of the atoms of the metal target. Then, electrons from higher states drop down to fill the vacancy, emitting characteristic x-ray photons (characteristic x-rays) with precise energies determined by the difference of the energy levels where the electron transition has occurred: $\Delta E = E_i - E_f = hf$ [11]. The wavelength λ , in pm, can be derived from the tabulated energy E , in keV, by the relationship: $E = hf$ $f = c/\lambda$ $E = hc/\lambda$ $\lambda = hc/E$ $\lambda(\text{pm}) = \frac{1239.81}{E(\text{keV})}$

If one plots the intensity of the x rays emitted versus the x rays wavelength for varying accelerating voltage, one obtains that the intensity increases with the energy voltage and with Z of anode. The maximum intensity is at $1.5\lambda_{\text{min}}$. This peak is characterized by a continuous distribution of radiation which becomes more intense and shifts toward higher frequencies or lower wavelengths when the energy voltage of the bombarding electrons is increased [11].

The general fall in the x-ray absorption coefficient or in the plot of the x-rays intensity versus the x-rays wavelength is interrupted by a sharp rise when the energy is equal to the binding energy of an electron shell (K, L, M, etc.) in the absorber [11]. This sharp rise is the minimum value of energy at which a vacancy can be created in the particular shell. It is referred as the 'edge' or 'critical excitation' energy. They are generated when a vacancy in an inner shell created by an X-ray or an electron excitation, is filled by the transfer of an electron from another shell, thus leaving another vacancy in that shell. At this process, it is emitted by the electron characteristic x-ray photons or spectral lines during the transition as it was mentioned before. The energy of the line is equal to the difference of the binding energies of the shells where the electron transition has occurred: $\Delta E = E_i - E_f = hf$. Depending on the atomic number, the X-ray spectra from the elements can include lines from the K, L, M, N and O series corresponding to excitation of the K, L, M, N or O levels. Lines are identified both by the common labels: $K\alpha_1$, $K\alpha_2$ for example or the term labels giving in order the shells with the 'initial' and 'final' vacancies: $KLII$, $KLIII$.

In the case of a metal with a small atomic number such as copper or molybdenum, we observe very characteristic lines [11]. They are caused by electrons being knocked out of the K shell of an atom and then the electrons from the L shell cascading down into the vacancies in this K shell. The energy emitted in this process corresponds to the so-called K_α ($n=2$ to $n'=1$) and K_β ($n=3$ to $n'=1$) lines. Transitions to the $n=2$ or L shell are designated as L x rays: $n=3$ to $n'=2$ is L_α , $n=4$ to $n'=2$ is L_β [11].

The continuous distribution of x rays which forms the base of the plot of the x rays intensity versus the x rays wavelength is the bremsstrahlung radiation (white radiation). The probability that a vacancy in a given shell will result in emission of an X-ray is the fluorescence yield of that shell. Not all vacancies result in the production of characteristic X-ray photons since there is a competing internal rearrangement process known as the Auger effect [11]. The ratio of the number of vacancies resulting in the production

of characteristic X-ray photons to the total number of vacancies created in the excitation process is called the fluorescent yield. The selection rules for the production of normal lines require that the principal quantum number n must change by at least one, the angular quantum number l must change by $(+,-)1$, and the J quantum number (where $J = l + s$, s is the spin quantum number) must change by 0 or 1.

In effect, this means that for the K series only p,s transitions are allowed, yielding two lines for each principal level change [11]. Vacancies in the L level follow similar rules and give rise to L series lines. There are more of the L lines since p,s, s,p and d,p transitions are all allowed [11]. In practice, the number of lines observed from a given element will depend upon the atomic number of the element, the excitation conditions and the wavelength range of the spectrometer employed. While most of the observed fluorescent lines are normal, certain lines which are called forbidden lines may also occur in X-ray spectra that do not at first sight fit the basic selection rules.

Other source of photons is the radioactivity. It refers to the particles which are emitted from the nucleus as a result of the nuclear instability. Because the nucleus supports the intense conflict between the two strongest forces in the nature (strong and electromagnetic forces), it should not be surprising that there are many nuclear isotopes which are unstable and emit some types of radiation. The most common types of radiation are called alpha, beta, and gamma radiation, but there are other varieties of radioactive decay. After a radioactive decay, the daughter-nucleus is often in an excited state and it can get into the ground-state by emitting a high energy gamma-photon. These photons can only have discrete energy values. The different types of radioactivity bring to different decay paths which transmute the nucleus into other chemical elements. It is possible to get mono-energetic x-rays photons with the decay product of Am(241) in Np (237).

4. Atom

4.1. Brown Research

In 1827, Brown observed that the pollen grains of the plants acquired some movement when entering the water. After 40 years, it was concluded that this movement was due to eventual collisions of small invisible particles that belonged to the liquid and not to the pollen. These particles were the atoms of the liquid that when colliding with the pollen particles were in evidence.

After, it was shown that these invisible water particles were not atoms but molecules, which in turn are composed of atoms. In this way, the atomic theory began to establish itself among scientists. This was an indirect observation. The atoms cannot be seen but with the microscope the movement of the pollen within the liquid can be observed due the movement of the atoms of the liquid. Thus, it is possible to study atoms indirectly even though they are not visible [8].

In 1905, Albert Einstein published an article where he explained in detail how the movement that Brown had observed was the result of micro particles being moved by individual water molecules [8]. This explanation served as convincing proof that atoms and molecules exist which was verified experimentally by Jean Perrin in 1908. Later, Perrin was awarded the Nobel Prize in Physics in 1926 for his work on the discontinuous structure of matter. Einstein had received the award five years earlier for his theoretical research of the Photoelectric Effect. Furthermore, Einstein made many contributions in atomic physics with ideas and theoretical research in the Blackbody Research of Planck and the quantization of the atom and the radiation field (light) at the Photoelectric Effect. Nevertheless, Einstein's biggest contribution was in Gravitation research about the Spatial and General Relativity.

4.2. Rutherford Model

The electrical field at the atom is very similar to the gravitational field at the Planetary System. In fact, it is possible to observe the analogy at the force formula for the atom and for the planetary system:

$$F = k \frac{e^2}{r^2} \quad F = G \frac{mM}{r^2}$$

At the planetary system, the gravitational force is the responsible for the motion of the Planets around the Sun. At the atom, the electrical force is the responsible for the motion of the electrons around the nucleus.

Fig.10. The electron orbiting around the nucleus

Rutherford proposed a microscopic planetary system: an electron with negative charge orbiting a nucleus with positive charge. The Rutherford Model was in agreement with the experiments of Geiger and Marsden where a N number of α particles which have positive charge hit a sheet of Gold, Aluminum or Cooper. After, a certain number of these α particles collide on the detector screen (detected as flashes) which was located at a determined angle [4]. A certain number of α particle was deviated by the interaction with the nucleus which has also a positive charge. The deviation is consequence of the electrical force of repulsion between the α particle and the nucleus. Therefore, this experiment only can be explained if the nucleus is constituted by a nucleus of positive charge with the electrons with negative charge moving around it at a large distance or radius respect to the nucleus [4], [5], [8]. Rutherford

obtained a formula (in agreement with Geiger and Marsden formula) for the number of the particles (number of flashes) which collides on the detector screen [4]:

$$f = \frac{NntZ^2e^4}{4R^2\left(\frac{1}{2}mv_o^2\right)^2 \sin^4\left(\frac{\Phi}{2}\right)}$$

N: number of α particles which hit the sheet of Gold e: electron charge

n: number of atoms by volume of the sheet Φ : angle deviation of α particles

Z: nucleus charge $K = \frac{1}{2}mv_o^2$: kinetic energy of the α particles

R: distance between the sheet and the detector screen t: thickness of the sheet

Nevertheless, the electromagnetic theory of Maxwell has established that an accelerated charged particle as the electron emits electromagnetic radiation (photons) during the accelerated motion [2]. Besides, the electron losses mass during the emission. At the Rutherford model, the electrons move around the nucleus with acceleration because the velocity direction is changing every time. Therefore, the electrons will radiate electromagnetic energy in a continue form. As consequence of it, the electrical force will put the electrons towards the core of the nucleus [4]. Besides, it will result in a continuous spectrum of energy emission of the electron and in instability of the atom (atom collapse) and the matter in general. But, it doesn't occur in the reality: there is a discrete spectrum of energy emission of the electron at the atom and there is stability at the atom. Then, it was necessary to obtain other model to explain this fact. After, Bohr proposed a model with some postulates to solve the instability of the atom.

4.3. Spectral Lines of the Atom

The radiation emitted by a blackbody is continuous because it contains energy of all frequencies [4], [5]. It was used electron oscillators at the cavity walls with emission of discrete energy (quantization) proposed by Planck to explain this continuous radiation at the region of low and high frequency. It is used the same energy quantization at the emission or absorption of energy by the electrons at the atom. It is because the blackbody radiation at the macroscopic scale is also emitted by electrons of the atoms at the walls of the blackbody. Then, it is evident that the same approach is possible to use to analyze the atom at the microscopic scale. Nevertheless, atoms (as Hydrogen for example) and other sources of elements (electric discharge in a sodium lamp or neon gas tube) emit discrete spectral lines of frequencies. By researching those spectral lines, it was possible to understand the internal structure of the atoms [4], [5]. Mendeleev established the periodic classification of the elements in the periodic table. The relation between the spectroscopy and the internal structure of the atoms was evident with this research [4], [5]. Then, Balmer found empirically a formula which described the experimental spectral lines of the Hydrogen. It was a proof of the internal structure of the atom and the energy emission of electrons when they jump from one energy level to another [4], [5]. The Balmer formula was very

important to test the Bohr Model. The formula found by Balmer is as follows: $\frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{n^2}\right)$

$$\lambda = 3645.6 \left(\frac{n^2}{n^2 - 2^2} \right) (\text{\AA})$$

$n=3, 4, 5, \dots$ $R=1.097313414 \times 10^7 \text{ m}^{-1}$: Rydberg constant

For $n=3$, the wavelength of the spectral line is $\lambda=6562.08 \text{ \AA}$. The experimental value of the spectral line is $6562.10 \text{ \AA}$. There is a good concordance between the experimental value and the Balmer formula. The regularity found at the Hydrogen Atom was discovered also in other elements of the periodic table [4], [5]. For example, Paschen found a formula for the spectral lines of the Hydrogen at the infrared zone of the spectrum [5]. After, it was found the Lyman and Brackett series for the ultraviolet and infrared zone of the spectrum [5]. Those formula are as follows:

$$\frac{1}{\lambda} = R\left(\frac{1}{3^2} - \frac{1}{n^2}\right) \quad n=4,5,6,\dots \text{ Paschen Serie}$$

$$\frac{1}{\lambda} = R\left(\frac{1}{1^2} - \frac{1}{n^2}\right) \quad n=2,3,4,\dots \text{ Lyman Serie}$$

$$\frac{1}{\lambda} = R\left(\frac{1}{4^2} - \frac{1}{n^2}\right) \quad n=5,6,7,\dots \text{ Brackett Serie}$$

Then, it was concluded that the discrete spectral lines can be adjusted by the formula [4], [5]: $\frac{1}{\lambda} =$

$$R\left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad \text{wavelength spectral lines } n > n'$$

$$f = cR\left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad c=\lambda f \quad \text{frequency spectral lines}$$

$$\Delta E = hcR\left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad \Delta E=hf \quad \text{energy spectral lines}$$

4.4. Bohr Model for the Hydrogen Atom, analogy with the blackbody cavity and reasons for the determined electron radius

In 1913, Bohr found a solution to explain the stability of the atom based in the hypothesis introduced by Planck (1900) at the Blackbody radiation. Besides, Einstein contributed with the approach of quantization for the light radiation at the Photoelectric Effect (1905) [4], [5], [9]. This research was about the quantization of the absorption, emission and transmission of the radiation energy. Then, Bohr introduced the concept of discrete quantum energy emission by the electrons at the atom with energy $\Delta E=hf$. It was analogous to the discrete energy emission (quantized energy) by the electron oscillators at the cavity of the Blackbody of Planck and the quantization of the radiation at the Photoelectric Research of Einstein. The postulates of Bohr are as follows:

1.- The electrons doesn't radiate energy in the stationary orbits around the nucleus. The electron is accelerated at the stationary orbits because the velocity changes the direction in the circular motion

around the atom. The classic electromagnetic theory of that accelerated electron radiates electromagnetic radiation is not applied.

2.- The electron only can orbit around the nucleus in stable orbits or stationary levels with constant energy. The electrons can change its orbit (which has a specific radius) when they emit or receive energy. Then, the atoms gain or lose energy when the electrons pass from one orbit to another.

3.- The energy of the photon emitted or absorbed by the electron at the transition from one orbit to another is equal to the energy difference between the respective energy of the electron orbits where has occurred the transition:

$$\Delta E = E_i - E_f = hf = hc/\lambda \quad \text{for emission energy } E_i > E_f \quad (E_i \text{ is less negative than } E_f)$$

Bohr could explain the atom stability with those postulates and obtain a formula for the quantization of the energy, velocity, radius, angular momentum, frequency and wavelength of the radiation emitted or absorbed [4], [5], [8], [9]. The quantization formula of Bohr [4], [5] is as follows: $\oint p \, ds = nh$ where
p: momentum $p = mv$

s: traveled distance of the electron around the nucleus: $ds = 2\pi dr$

h: Planck Constant n : integer number: main quantum (level) number

Bohr also postulated a quantization for the angular momentum: $L = \frac{nh}{2\pi}$

Nevertheless, those postulates did not explain why there is no emission of radiation when the electrons orbit around the nucleus. Later, it could be explained by using the approach of De Broglie wave-particle duality. The experiment of Franck Hertz was other proof (in addition of the Blackbody radiation and the Photoelectric Effect) of the existence of stationary states in the atom and the Bohr model and postulates. The experiment consisted in the process of excitation and de-excitation of a gas sample. This is utilized the electroluminescence phenomenon. There is a filament F that emits electrons that are accelerated towards a grating by means of a variable potential V. The space between the filament and the grating is occupied by mercury vapor (gas). A small potential difference is applied between the grating and the plate where it is measured the current. Due to the polarity of this potential, the electrons are decelerated and the current in the plate is measured with the galvanometer [4].

When the accelerated electrons do not have enough energy to bring the atomic system to an excited state, they pass through the region between the filament and the grating, losing a minimum part of their energy and the current measured in the galvanometer has a large value. If the energy of the electrons is greater than or equal to the difference between the energies of the ground state and the first excited state, the electron will lose much of its energy which will be converted into excitation energy of the atomic system.

The current measured in the galvanometer will be very low since fewer electrons will arrive per time unit [4].

Fig.11. Franck-Hertz Experiment: Graph of current intensity versus voltage

By increasing the accelerating potential, the energy of the electrons will have a value that after causing an excitation will have enough energy left to cause more excitations. The current measured in the galvanometer will drop further [4]. The first valley V_1 in the graph corresponds to the electrons that lose almost all of the kinetic energy in one interaction. The second valley V_2 in the graph corresponds to the second excitation of the electrons that has excited two atoms [4]. Due to the tendency of every atom to be in its fundamental or stationary state, the energy transferred from the electron to the atom is emitted by the atom in the form of radiation [4]. This can be calculated by measuring the wavelength of the emitted light and calculating its energy: $\Delta E = hc/\lambda$ $\Delta E = hf$ $c = \lambda f$.

The difference in energy between the ground state and the first excited state according to Bohr postulate is: $\Delta E = E_1 - E_2 = \frac{hc}{\lambda}$. The spectroscopy result is $\Delta E = 4.86$ eV. This corresponds to the energy emitted by the atom to return to its fundamental state [4]. The experimental result is 4.9 eV which is possible to observe at the graphic. Thus, it is required an accelerating potential of 4.9 V for the electron to cause an atomic excitation of 4.9 eV [4]. This coincidence between the values of the energy of the emitted radiation and the electron energy necessary (potential difference or voltage) to achieve an excitation is an evident and clear proof of the existence of stationary states in the atom and the Bohr model and the postulates [4]. This experiment is similar to the Photoelectric Effect but instead of light radiation incident, it is used electrons. As the light, the electrons can give their energies as discrete packet of energy when it is greater than or equal to the energy difference between the energies of the ground state and the first excited state. The lost energy of the electron is converted into excitation energy of the atomic system as at the Photoelectric Effect. There is analogy of the atom with the blackbody research from Planck and harmonic oscillators. The electromagnetic radiation at temperature T inside a cubic shaped cavity with L-edge and metal is studied at the blackbody cavity. The allowed electromagnetic waves have wavelength $(2n+1)\lambda = L$ with n an integer (the electric field must be zero at the walls) [3]. The

cavities corresponds to the respective orbits at the atom. Then, the correspondence analogy with the atom is as follows:

$$\lambda = a_0 \quad L = \Delta r$$

$$(2n+1)\lambda = L \quad (2n+1) a_0 = \Delta r$$

$$r_1 - r_0 = (2n+1) a_0 \quad r_0 = a_0$$

$$r_1 = a_0 + (2n+1) a_0 \quad r_1 = 4 a_0 \quad n=1$$

$$r_2 = r_1 + (2n+1) a_0 \quad r_2 = 4 a_0 + (2n+1) a_0 \quad n=2 \quad r_2 = 9 a_0$$

Then, the formula for the radius of the electron orbit at the atom is as follows:

$$r_n = n^2 a_0$$

This formula is in concordance with the quantization formula obtained by applying the postulates of Bohr and the De Broglie duality.

Besides, it is possible to explain why the electron has determined stationary radius at the atom. The planets are orbiting around the Sun due the gravitational field in the planetary system. The curvature of the space-time causes the motion of the planets as it is explained in General Relativity. Also, there is a perihelium precession of the Mercury orbit due the high relativistic velocity and the strong curvature or field between Mercury and the Sun. At the atom, the electrons are orbiting around the nucleus due the electrical field. The electrical field determines the restricted radius at the atom. In addition, there is also a precession motion of the electron orbits due the high relativistic velocity.

4.5. De Broglie duality: no energy radiation for electron as wave

De Broglie established that the matter has properties of wave and particle. It is in accordance with the symmetry property of the Universe. Thus, the waves have properties of particles and the particles have properties of waves: wave-particle duality [4], [5], [9]. The formula that relates the mass of the particle and the wavelength of the wave is as follows: $\lambda = \frac{h}{mv}$

$$E^2 = p^2 c^2 + m_0^2 c^4 \quad \text{Relativistic Dirac equation} \quad \text{For light } m_0=0$$

$$E^2 = p^2 c^2 \quad E = hf \quad hf = pc \quad f = c/\lambda \quad \frac{h c}{\lambda} = pc$$

$$p = \frac{h}{\lambda} \quad \text{momentum for a wave}$$

$$p = mv \quad \text{momentum for a particle}$$

$$mv = \frac{h}{\lambda} \quad \lambda = \frac{h}{mv} \quad \text{De Broglie wavelength for a particle}$$

Therefore, the electron has properties of waves with De Broglie wavelength which satisfied the Wave Schrödinger Probabilistic Equation. At the Schrödinger Approach, the position (electron region), momentum and energy of the electron are probabilistic (no definite). Other approach is that the electrons are guided by a pilot wave like a surfer on a wave. At this approach, every electron always has a definite position like the surfer: an electron is pushed or guided by a guiding pilot wave which influences the electron's location. It is a new interpretation of quantum mechanics.

It is possible to explain the postulate of Bohr. The electron moves around the nucleus in a perimeter equal to $2\pi r$. At the stationary level, the wavelength of the electron is equal to the distance traveled by the electron $2\pi r$. If $2\pi r$ is not equal to this wavelength, then the electron needs to move to other orbit where $2\pi r = n\lambda$. It corresponds to other stationary level for the electron and n is the orbit number $n=1,2,3,\dots$ [4], [5], [9].

Fig.12. Motion of the wave electron by adjustment of De Broglie waves

It is the reason that the electron doesn't radiates energy at the stationary level: the electron doesn't have additional energy $E=hf$ to radiate. All of its energy E corresponds to the mass-energy equivalent of the electron ($E=mc^2$) at the stationary level with $m = \frac{h}{\lambda v}$ where λ and v are constant ($\lambda=2\pi r$): m constant.

Thus, if the electron receives additional energy or losses energy, the electron cannot remain in this orbit because the electron has other energy E which correspond to other wavelength $\lambda=hc/E$ (other radius r) and other mass-energy equivalent $m=E/c^2$. As consequence of it, the wavelength λ is not equal to $2\pi r$ at this orbit anymore. Then, the electron does the transition to other stationary where $n\lambda=2\pi r$ ($n=1,2,3,\dots$) with the emission of electromagnetic radiation or photons. The new stationary orbit for the electron with other radius r has other velocity and so, there is a new wavelength $\lambda = \frac{h}{mv}$ for the electron. Besides, the vacancy left in the atomic structure by the ejected electron due the energy absorption at the photoelectric effect is filled by one of the electrons from a higher shell or by a free electron from outside the atom. This transition is accompanied by the emission of a photon. This transition occur without energy absorption of the electron of the higher shell. It is because the atoms and the matter always prefer and change their state to a stationary level or minimum energy after an excited level. It is other principle or law of our universe as the symmetry properties.

The wave properties of macroscopic objects are not evident because they have a very small wavelength ($E=hc/\lambda$: high energies and $f=c/\lambda$: high frequencies). At the atomic scale, the electron wavelength is not so small and its wave behavior can be observed. In 1927, Davisson and Germer verified the wave character of the electrons by means of an electron diffraction experiment [5].

The electrons emitted by a metallic filament are accelerated through the potential difference ΔV and then, they are impinged on a nickel crystal [5]. By applying the law of energy conservation, this is possible to obtain:

$$K=U=e\Delta V \quad K = \frac{1}{2}mv^2 = \frac{p^2}{2m} = e\Delta V \quad U: \text{ potential energy } V: \text{ voltage}$$

$$p = \sqrt{2me\Delta V} \quad \lambda = \frac{h}{p} = \frac{h}{\sqrt{2me\Delta V}} \quad \text{De Broglie wave}$$

By replacing the values of h , m , e and $\Delta V=150$ V, the wavelength is $\lambda=1$ Å. A crystal can diffract x-rays with wavelength of 1 Å. This diffraction is due to the fact that the crystal contains defined planes which are called Bragg planes where the atoms are located [5], [13]. For the case of light wave, the reflected light in the Bragg planes interferes constructively with the condition that the difference in travel distance between neighboring planes is equal to an integer number of wavelengths [5], [13]. The Bragg formula is as follows: $n\lambda=2d\sin\theta$. This formula that is applicable for the light would be also valid for electrons if they also behave as waves [5]. The detector was found to measure an angle of $\Phi=50^\circ$, $\Phi+2\theta=180^\circ$, $\theta=65^\circ$, with a voltage of $\Delta V=54$ V.

Fig.13. Electron Diffraction

Since the spacing of the reflective Bragg planes of the crystal was $d=0.91$ Å and $n=1$, the wavelength was: $\lambda=2(0.91)\sin(65)=1.65$ Å. De Broglie wave was: $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2me\Delta V}} \quad \Delta V=54$ V $\lambda=1.67$ Å.

The experiment of Davisson and Germer demonstrated that electrons diffract and behave like waves as the De Broglie wave-particle duality has predicted. In 1927, Thomson also confirmed the electron diffraction [5]. In 1929, Estermann and Stern confirmed experimentally that helium and hydrogen molecules also diffracted according to De Broglie's theory. Later, neutrons were also found to be

diffracted according to De Broglie. It showed that the wave-particle duality is for all particles: both matter and light can have corpuscular and wave behavior [5].

By applying the wave-particle duality of De Broglie to the electron, it is possible to obtain the quantization of the angular momentum and the Bohr Postulate [4], [5]. The electron behaves like a wave and only a whole number of wavelengths can fit in the Bohr orbit: $n\lambda = 2\pi r$ $n=1,2,3,\dots$

$$\lambda = \frac{h}{mv} \quad \text{De Broglie wavelength}$$

$$n \frac{h}{mv} = 2\pi r \quad nh = 2\pi mvr \quad p=mv$$

$$nh=2\pi pr \quad nh=2\pi L \quad L=pr$$

$$L = \frac{nh}{2\pi} \quad \text{Bohr Angular Momentum} \quad n=1,2,3,\dots$$

$$nh = 2\pi mvr \quad mv2\pi r = nh \quad p=mv \quad s=2\pi r \quad ds=2\pi dr$$

$$\oint pds = nh \quad \text{Bohr Postulate} \quad n=1,2,3,\dots$$

4.6. Quantization Formula and Rydberg constant deduction

$$m \frac{v^2}{r} = \frac{kZe^2}{r^2} \quad r = k \frac{Ze^2}{mv^2} \quad \text{where } k=1/(4\pi\epsilon_0) \quad k=9 \times 10^9 \text{ N-m}^2/\text{C}^2$$

$$n\lambda = 2\pi r \quad \lambda = \frac{h}{mv} \quad \text{De Broglie wave and adjustment of waves at the orbit}$$

$$n \frac{h}{mv} = 2\pi r \quad r = \frac{nh}{2\pi mv}$$

$$\frac{nh}{2\pi mv} = k \frac{Ze^2}{mv^2} \quad k=1/(4\pi\epsilon_0)$$

$$v = \frac{Ze^2}{2\epsilon_0 nh} \quad \text{Quantization of the velocity}$$

$$r = \frac{nh}{2\pi mv}$$

$$r = \frac{\epsilon_0 h^2}{\pi m Ze^2} n^2 \quad \text{Quantization of the radius } a_0 = \frac{\epsilon_0 h^2}{\pi m e^2} = 0,529 \text{ A Bohr radius}$$

$$E=K+U \quad \text{Total Energy for the electron at the atom}$$

$$E = \frac{1}{2}mv^2 - \frac{kZe^2}{r} \quad m \frac{v^2}{r} = \frac{kZe^2}{r^2} \quad \frac{1}{2}mv^2 = \frac{kZe^2}{2r}$$

$$E = \frac{kZe^2}{2r} - \frac{kZe^2}{r}$$

$$E = -\frac{kZe^2}{2r} \quad \text{Total Bound Energy for the electron at the atom}$$

$$r = \frac{\epsilon_0 h^2}{\pi m Z e^2} n^2 \quad k=1/(4\pi\epsilon_0)$$

$$E = -\frac{mZ^2 e^4}{8\epsilon_0^2 n^2 h^2} \quad \textbf{Quantization of the energy}$$

$$L=pr \quad L=mvr$$

$$v = \frac{Ze^2}{2\epsilon_0 nh} \quad r = \frac{\epsilon_0 n^2 h^2}{\pi m Z e^2}$$

$$L=m \frac{Ze^2}{2\epsilon_0 nh} \frac{\epsilon_0 n^2 h^2}{\pi m Z e^2}$$

$$L=\frac{nh}{2\pi} \quad \textbf{Quantization of the angular momentum}$$

If the electron jumps from one orbit to another, the absorption or emission of the energy is equal to the energy difference between the two levels of energy where the transition has occurred. At the Planck Research, it was established that the energy is emitted as packets of discrete energy $\Delta E=hf$ due the electron oscillators at the cavity. At the atom, the energy is also emitted as packets of discrete energy $\Delta E=hf$. The proportional constant is the Planck Constant h . Therefore, there is analogy between the blackbody radiation and the atom radiation. If the radiation is emitted, the formula is $\Delta E=E-E'=hf$.

E : energy of the initial level or orbit: E is less negative than E'

E' : energy of the final level or orbit: $E>E' \quad |E'| > |E|$

n : quantum number of the initial level or orbit

n' : quantum number of the final level or orbit $n>n'$ for energy emission

$$E = -\frac{mZ^2 e^4}{8\epsilon_0^2 n^2 h^2} \quad E' = -\frac{mZ^2 e^4}{8\epsilon_0^2 n'^2 h^2} \quad \Delta E = E - E'$$

$$\Delta E = \frac{mZ^2 e^4}{8\epsilon_0^2 h^2} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad \textbf{discrete spectral lines for the energy emission}$$

It is possible to compare this formula with the Balmer formula ($Z=1$) of frequency and to conclude which factors are the Rydberg constant and to obtain the quantization energy formula of Bohr:

$$\Delta E = \frac{me^4}{8\epsilon_0^2 h^2} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad f = cR \left(\frac{1}{n'} - \frac{1}{n^2} \right) \quad R = \frac{me^4}{8\epsilon_0^2 ch^3} \quad \Delta E = hf$$

$$\Delta E = hf = \frac{mZ^2 e^4}{8\epsilon_0^2 h^2} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right)$$

$$f = \frac{mZ^2 e^4}{8\epsilon_0^2 h^3} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad \textbf{frequency spectral lines for energy emission } n>n'$$

$$\frac{c}{\lambda} = \frac{mZ^2 e^4}{8\epsilon_0^2 h^3} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad c=\lambda f$$

$$\frac{1}{\lambda} = \frac{mZ^2e^4}{8\varepsilon_0^2ch^3} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad \text{wavelength spectral lines for energy emission } n > n'$$

If the frequency formula is compared with the Balmer series ($Z=1$), it is possible to obtain the Rydberg Constant:

$$f = cR \left(\frac{1}{n'} - \frac{1}{n^2} \right) \quad f = \frac{mZ^2e^4}{8\varepsilon_0^2h^3} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad Z=1$$

$$cR = \frac{me^4}{8\varepsilon_0^2h^3} \quad R = \frac{me^4}{8\varepsilon_0^2ch^3} \quad \text{Rydberg Constant}$$

By replacing the values of m , e , ε_0 , c , h the Rydberg Constant is:

$$R = 1.097 \cdot 10^7 \, m^{-1}: \text{Rydberg Constant}$$

$$\Delta E = hf = \frac{mZ^2e^4}{8\varepsilon_0^2h^2} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad \Delta E = hf = hcRZ^2 \left(\frac{1}{n'^2} - \frac{1}{n^2} \right)$$

The agreement between the Balmer formula (empirical and experimental formula) and the Bohr formula (formula obtained from the Bohr Postulate) implies the concordance between the theory and the experimental data.

It is possible to obtain the Rydberg constant and the quantization formula ($Z=1$) based in the period of the electron around the nucleus:

$$v = \frac{2\pi r}{T} \quad v^2 = \frac{4\pi^2 r^2}{T^2} \quad T = 1/f_r \quad f_r: \text{revolution frequency of the electron}$$

$$E = K + U \quad E = \frac{1}{2}mv^2 - \frac{ke^2}{r}$$

$$m \frac{v^2}{r} = \frac{ke^2}{r^2} \quad mv^2 = \frac{ke^2}{r} \quad \frac{1}{2}mv^2 = \frac{ke^2}{2r}$$

$$E = \frac{1}{2}mv^2 - mv^2 \quad E = \frac{ke^2}{2r} - \frac{ke^2}{r}$$

$$E = -\frac{1}{2}mv^2 = -K \quad \text{or} \quad E = -\frac{ke^2}{2r}$$

$$\frac{2E}{m} = v^2 \quad E \text{ in absolute value} \quad \frac{2E}{m} = \frac{4\pi^2 r^2}{T^2} \quad T = 1/f_r$$

$$\frac{2E}{m} = 4\pi^2 r^2 f_r^2 \quad \frac{\sqrt{2}\sqrt{E}}{2\pi r \sqrt{m}} = f_r \quad E = \frac{ke^2}{2r} \quad r = \frac{ke^2}{2E} \quad k = 1/(4\pi\varepsilon_0)$$

$$f_r = \frac{4\varepsilon_0 \sqrt{2} E^{3/2}}{e^2 \sqrt{m}} \quad \text{revolution frequency of the electron}$$

$$\Delta E = hcR \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad E_n = -\frac{chR}{n^2} \quad |E_n| = \frac{chR}{n^2}$$

$$f_r = \frac{4\epsilon_0\sqrt{2}(chR)^{3/2}}{e^2\sqrt{mn^3}}$$

$$f = cR\left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad n > n' \quad \text{Balmer Series} \quad \text{for } n' = n-1, \text{ it is obtained:}$$

$$f = cR\left(\frac{1}{(n-1)^2} - \frac{1}{n^2}\right) \quad f = cR\left(\frac{2n-1}{(n-1)^2n^2}\right) \quad f_c = cR\frac{2}{n^3} \quad n \gg 1$$

For values of n very large in comparison with 1 (classic continuous where f is very small that the discrete lines can be not observed and ΔE is also very small), f_c is: $f_c = cR\frac{2}{n^3}$ $R = \frac{me^4}{8\epsilon_0^2ch^3}$ $f_c = \frac{me^4}{4\epsilon_0^2h^3n^3}$

It is the continuous region which occurs for quantum numbers n very large where the levels of energy are so close that they form a continuous region and the process is almost continuous and no discrete [9]. Then, this classic result must be in concordance with the formula development for the revolution frequency of the electron for the classic case $f_r = f_c$. It means that for quantum numbers very large, the frequency of the radiation emitted by the electron is equal to the revolution frequency of the electron as the classic electrodynamic predicts [9]: $f_c = f_r$ $cR\frac{2}{n^3} = \frac{4\epsilon_0\sqrt{2}(chR)^{3/2}}{e^2\sqrt{mn^3}}$ for quantum numbers very large

$$R = \frac{me^4}{8\epsilon_0^2ch^3}$$

By replacing this value in the energy formula, it is obtained:

$$E_n = -\frac{chR}{n^2} \quad E_n = -\frac{me^4}{8\epsilon_0^2n^2h^2} \quad \text{quantization of the electron energy}$$

$$\Delta E = E - E' = \frac{me^4}{8\epsilon_0^2h^2}\left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad \text{spectral emission energy} \quad n > n'$$

$$f = cR\left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad f = \frac{me^4}{8\epsilon_0^2h^3}\left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad \text{frequency of the energy emission}$$

$$\Delta E = hf = \frac{me^4}{8\epsilon_0^2h^2}\left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad \text{spectral emission energy}$$

$$f_r = \frac{4\epsilon_0\sqrt{2}(chR)^{3/2}}{e^2\sqrt{mn^3}} \quad f_r = f_c = cR\frac{2}{n^3} = \frac{me^4}{4\epsilon_0^2h^3n^3} \quad \text{electron revolution frequency}$$

$$r = \frac{ke^2}{2E} \quad E_n = -\frac{me^4}{8\epsilon_0^2n^2h^2} \quad k = \frac{1}{4\pi\epsilon_0}$$

$$r = \frac{n^2\epsilon_0h^2}{\pi me^2} \quad r = n^2a_0 \quad \text{radius quantization} \quad a_0 = \frac{\epsilon_0h^2}{\pi me^2} \quad \text{Bohr radius}$$

$$K = |E| \text{ in absolute value } \frac{1}{2}mv^2 = K = \frac{ke^2}{2r} \quad E = -\frac{ke^2}{2r} \quad V = -\frac{ke^2}{r} = -2K$$

$$E = -\frac{me^4}{8\epsilon_0^2n^2h^2} \quad K = \frac{me^4}{8\epsilon_0^2n^2h^2} \quad V = -\frac{me^4}{4\epsilon_0^2n^2h^2}$$

Other form to obtain the same formula is as follows: during the bound process of the electron ($n_i \gg n_f$), it is emitted radiation energy $V = nhf_c$ ($n_f = n$) of frequency f_c (due the electrical potential energy) equal to the double of the kinetic energy of the electron $2K$ in the final orbit or level [1].

K : kinetic energy of the electron n_i : initial level $n_f = n$: final level

$V = nhf_c$: potential energy: emission energy due the process of bound of the electron where $n_i \gg n_f$, $E_{ni} \approx 0$. This emission energy corresponds for $\Delta n = n_i - n_f$ very large.

It is the continuous region (large quantum numbers) where the levels of energy are so close that they form a continuous region.

Then, the spectral emission frequency f_c must be equal to the revolution frequency of the electron f_r at the final state for this continuous region $f_c = f_r$.

$$K = V/2 \quad K = nhf_c/2 \quad f_c = 2K/(nh)$$

$$v = \frac{2\pi r}{T} \quad v^2 = \frac{4\pi^2 r^2}{T^2}$$

$$\frac{1}{2}mv^2 = K \quad \frac{2K}{m} = v^2$$

$$\frac{2K}{m} = \frac{4\pi^2 r^2}{T^2} \quad \frac{2K}{m} = 4\pi^2 r^2 f_r^2 \quad T = 1/f_r$$

$$\frac{\sqrt{2}\sqrt{K}}{2\pi r\sqrt{m}} = f_r \quad K = \frac{ke^2}{2r} \quad r = \frac{ke^2}{2K} \quad k = 1/(4\pi\epsilon_0)$$

$$f_r = \frac{4\epsilon_0\sqrt{2}K^{3/2}}{e^2\sqrt{m}} \quad f_c = f_r \quad \text{for } \Delta n = n_f - n_i \text{ large}$$

$$\frac{2K}{nh} = \frac{4\epsilon_0\sqrt{2}K^{3/2}}{e^2\sqrt{m}}$$

$$K = \frac{me^4}{8\epsilon_0^2 n^2 h^2} \quad E = -K \quad E = -\frac{me^4}{8\epsilon_0^2 n^2 h^2}$$

$$\Delta E = E - E' = hf = \frac{me^4}{8\epsilon_0^2 h^2} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad \text{spectral emission energy}$$

$$f = \frac{me^4}{8\epsilon_0^2 h^3} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad \text{frequency of the energy emission}$$

$$f_r = \frac{4\epsilon_0\sqrt{2}K^{3/2}}{e^2\sqrt{m}} \quad K = \frac{me^4}{8\epsilon_0^2 n^2 h^2} \quad f_r = \frac{me^4}{4\epsilon_0^2 h^3 n^3}$$

$$f_c = 2K/(nh) \quad f_c = \frac{me^4}{4\epsilon_0^2 h^3 n^3} \quad f_r = f_c$$

$$r = \frac{ke^2}{2K} \quad K = \frac{me^4}{8\epsilon_0^2 n^2 h^2} \quad r = \frac{n^2 \epsilon_0 h^2}{\pi m e^2} \quad r = n^2 a_0 \quad a_0 = \frac{\epsilon_0 h^2}{\pi m e^2}$$

4.7. Correction of the nuclear mass

It is necessary for a better agreement with the experimental results to take in account the finite mass of the nucleus and its effect at the motion of the electron [9]. It is possible to apply momentum conservation:

$$mv = MV \quad V = (m/M)v \quad m: \text{mass of the electron} \quad M: \text{mass of the nucleus}$$

$$K_M = \frac{1}{2}MV^2 = \frac{1}{2}\frac{m^2}{M}v^2 = \frac{m}{M}K \quad \text{where } K = \frac{1}{2}mv^2$$

If M has a very high value $M \gg m$ (nucleus with infinite mass), then K_M is negligible and the nucleus can be considered as fixed. If it is considered the finite mass of the nucleus, then it is possible to consider the nucleus also as fixed but the electron mass is the reduced mass of the system μ instead of m [9]. The formula for the reduced mass is obtained by applying the conservation rule for the kinetic energy for the two cases: the electron with mass equal to the reduced mass μ moving around the fixed nucleus and the electron moving around the center of mass with the nucleus also moving around the center of mass which also occurs in binary stars.

$$K = \frac{1}{2}mv^2 = \frac{p^2}{2m} \quad p = mv \quad p: \text{electron momentum} \quad P: \text{nucleus momentum}$$

$$p = P \quad mv = MV \quad \text{where } v \text{ is the electron velocity and } V \text{ is the nucleus velocity}$$

The conservation rule for the kinetic energy is as follows:

$$\frac{p^2}{2\mu} = \frac{p^2}{2m} + \frac{p^2}{2M} \quad \frac{1}{\mu} = \frac{1}{m} + \frac{1}{M} \quad \mu = m\left(\frac{M}{m+M}\right)$$

It is possible to do the analysis for the center of mass (CM) as follows:

Fig.14. Electron and nucleus orbiting around the common center of mass

By considering the center of mass in $r=0$, it is obtained:

$$mr = MR \quad R = (m/M)r \quad r' = r + R \quad r' = r + (m/M)r$$

$$r' = \frac{M+m}{M}r \quad r' = \frac{m}{\mu}r \quad r = \frac{M}{M+m}r' \quad r = \frac{\mu}{m}r'$$

$$L = \mu v r' = m \left(\frac{M}{m+M} \right) v \frac{M+m}{M} r = mvr \quad L = \mu v r' = mvr = n \frac{h}{2\pi}$$

$$L = pr = mvr = mv \frac{M}{M+m} r' = \frac{mM}{(M+m)} vr' = \mu vr' \quad L = mvr = \mu vr' = n \frac{h}{2\pi}$$

It is possible to obtain all the quantization formulas by replacing μ by m and the nucleus is at fixed position and at distance r' from the electron.

$$\mu vr' = n \frac{h}{2\pi} \quad n=1,2,3,\dots \quad r' = \frac{nh}{2\pi\mu v} \quad \mu = \frac{mM}{(M+m)}$$

$$\mu \frac{v^2}{r'} = k \frac{e^2}{r'^2} \quad r' = k \frac{e^2}{\mu v^2} \quad \frac{nh}{2\pi\mu v} = k \frac{e^2}{\mu v^2} \quad k=1/(4\pi\epsilon_0)$$

$$v = \frac{e^2}{2\epsilon_0 nh} \quad \textbf{Quantization of the velocity}$$

$$r' = \frac{nh}{2\pi\mu v} \quad v = \frac{e^2}{2\epsilon_0 nh}$$

$$r' = \frac{\epsilon_0 h^2}{\pi \mu e^2} n^2 \quad \textbf{Quantization of the radius}$$

$$r = \frac{\mu}{m} r' \quad r = \frac{\epsilon_0 h^2}{\pi m e^2} n^2 \quad a_0 = \frac{\epsilon_0 h^2}{\pi m e^2} \quad \text{Bohr radius}$$

If we consider the electron moving around the center of mass CM, it is possible to obtain the radius r as follows: $mw^2r = k \frac{e^2}{r'^2} = k \frac{e^2}{r^2} \frac{\mu^2}{m^2} \quad r' = \frac{m}{\mu} r$

It is possible to obtain the same equation as before by replacing:

$$mw^2r = mw^2 \frac{\mu}{m} r' = \mu w^2 r' = \mu \frac{v^2}{r'} = k \frac{e^2}{r'^2} \quad v = wr' \quad r' = \frac{m}{\mu} r$$

$$L = \mu vr' = \mu (r'w) r' = \mu wr'^2 = m \left(\frac{M}{M+m} \right) w \left(\frac{M+m}{M} \right)^2 r^2 = m \frac{M+m}{M} wr^2 = n \frac{h}{2\pi}$$

$$m \frac{M+m}{M} wr^2 = n \frac{h}{2\pi}$$

$$m \frac{M+m}{M} wr^2 = m \frac{m}{\mu} wr^2 = n \frac{h}{2\pi} \quad w = \frac{nh\mu}{2\pi m^2 r^2}$$

By replacing w in the force equation: $mw^2r = k \frac{e^2}{r'^2} = k \frac{e^2}{r^2} \frac{\mu^2}{m^2}$, it is obtained:

$$m \left(\frac{nh\mu}{2\pi m^2 r^2} \right)^2 r = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r^2} \frac{\mu^2}{m^2} \quad k = \frac{1}{4\pi\epsilon_0}$$

$$r = \frac{\epsilon_0 h^2}{\pi m e^2} n^2 \quad w = \frac{\pi e^4 \mu}{2 n^3 h^3 \epsilon_0^2} \quad r' = \frac{m}{\mu} r \quad r' = \frac{\epsilon_0 h^2}{\pi \mu e^2} n^2$$

$$r' = \frac{nh}{2\pi\mu v} \quad v = \frac{nh}{2\pi\mu r'} \quad v = \frac{e^2}{2\epsilon_0 nh}$$

$$v = r'w = \frac{m}{\mu} r w = \frac{m}{\mu} \frac{\epsilon_0 h^2}{\pi m e^2} n^2 \frac{\pi e^4 \mu}{2 n^3 h^3 \epsilon_0^2} \quad v = \frac{e^2}{2\epsilon_0 nh}$$

$$E = -\frac{ke^2}{2r'} \quad \text{Total Bound Energy for the electron at the atom}$$

$$r' = \frac{\epsilon_0 h^2}{\pi \mu e^2} n^2 \quad k=1/(4\pi\epsilon_0)$$

$$E = -\frac{\mu e^4}{8\epsilon_0^2 n^2 h^2} \quad \text{Quantization of the energy}$$

$$L=pr=mvr= \mu vr' \quad v = \frac{e^2}{2\epsilon_0 nh} \quad r' = \frac{\epsilon_0 n^2 h^2}{\pi \mu e^2}$$

$$L=\mu \frac{e^2}{2\epsilon_0 nh} \frac{\epsilon_0 n^2 h^2}{\pi \mu e^2} \quad L=\frac{nh}{2\pi} \quad \text{Quantization of the angular momentum}$$

$$\Delta E=E-E'=hf=\frac{\mu e^4}{8\epsilon_0^2 h^2} \left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad E>E' \quad (E \text{ is less negative than } E') \quad n>n'$$

$$f = \frac{\mu e^4}{8\epsilon_0^2 h^3} \left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad \text{spectral lines for the frequency for energy emission}$$

$$\Delta E = h \frac{\mu e^4}{8\epsilon_0^2 h^3} \left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad \Delta E = \frac{\mu e^4}{8\epsilon_0^2 h^2} \left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad \text{energy emission}$$

$$\frac{c}{\lambda} = \frac{\mu e^4}{8\epsilon_0^2 h^3} \left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad c=\lambda f$$

$$\frac{1}{\lambda} = \frac{\mu e^4}{8\epsilon_0^2 ch^3} \left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad \text{spectral lines for the wavelength for energy emission}$$

If this formula is compared with the Balmer series, it is possible to obtain the Rydberg Constant for the nuclear mass finite:

$$\frac{1}{\lambda} = R_M \left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad R_M: \text{ Rydberg constant for the nuclear mass finite}$$

$$\frac{f}{c} = R_M \left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad f = cR_M \left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \quad f = \frac{\mu e^4}{8\epsilon_0^2 h^3} \left(\frac{1}{n'^2} - \frac{1}{n^2}\right)$$

$$cR_M = \frac{\mu e^4}{8\epsilon_0^2 h^3}$$

$$R_M = \frac{\mu e^4}{8\epsilon_0^2 ch^3} \quad \text{Rydberg Constant for the nuclear mass finite}$$

$$R_M = \frac{\mu}{m} R \quad R: \text{ Rydberg constant for the infinite nuclear mass}$$

$$R = \frac{me^4}{8\epsilon_0^2 ch^3} \quad \mu = m \left(\frac{M}{m+M}\right)$$

$$R_M = \frac{M}{m+M} R = \frac{1836}{1837} R \quad M=1836 m \quad \text{where } m \text{ is the electron mass}$$

By replacing the values of m , e , ϵ_0 , c , h , the Rydberg Constant is:

$$R=1.097 \cdot 10^7 \text{ m}^{-1}: \text{ Rydberg Constant} \quad R_M=1.09678 \cdot 10^7 \text{ m}^{-1}$$

4.8. Quantum Numbers (n, l, m_l, m_s)

One of the most important advance at the research about the atom was the discover of the fine structure of the spectrum. It was evident that the spectral lines that appeared as one line with low precision equipment were in reality a set or group of lines very near among them with better spectroscopy equipment [4]. The electron state can be defined by the four quantum numbers: n, l, m_l and m_s [4], [5].

n : main quantum number which defines the electron energy, the lineal momentum, the electron velocity and the radius of the orbit. This number was introduced by Bohr for the quantization of the main energy levels. It is related with the magnitude of the volume occupied by the orbital which is the probable region where the electron is located. Also, this number takes in account the position of the electron around the nucleus at the ellipse approach ($r=a_0n^2$) and the revolution velocity of the electron at the orbit [8]. Besides, this number n is due the lineal momentum p of the electron at the Bohr Postulate: $\oint p ds = nh$. n : main quantum number $n=1,2,3,\dots$

l : orbital or azimuthal quantum number which defines the form and side of the orbital and the angular momentum. This number takes in account the form of the displacement of the electron around the nucleus at the ellipse approach by using the angular momentum L . The form of the displacement depends of the high relativistic velocity of the electron which causes the orbit precession. Therefore, it is necessary to apply Relativity Theory to the electron motion at the atom. As the angular momentum L describes the form of the electron orbit, the number l which is used for the quantization of the angular momentum makes restrictions to the possible orbits or sub-levels [4]. Then, new energy sub-levels were evident which were called spectrum of the fine structure or energy of fine structure.

In 1916, Wilson and Somerfield found a general rule to explain the quantization of the Planck energy of an oscillator and the Bohr quantization for the angular momentum. Somerfield considered elliptical orbits, the orbit precession and relativistic velocities for the electron with the introduction of a new quantum number l and new energy sub-levels. It could explain the new energy sub-levels or structure fine observed in the spectral lines. Nevertheless, the Bohr and Somerfield theories were useful only for simple systems with atoms with few electrons. But, it was an advance to stablish later the quantum theory of Schröndiger and Heisenberg [9].

The rule of Wilson and Somerfield is as follows: $\oint p_q dq = n_q h$, where the integral is on a complete cycle of the periodic motion of the electron, n_q is an integer quantum number, p is the momentum associated with the coordinate q . For example, for the one dimensional harmonic oscillator, the coordinate q is x and the momentum is p_x . For a circular motion, the coordinate q is θ and p_q is L : the angular momentum or q is $s=2\pi r$ and the momentum is p_s .

This consideration of the ellipse approach for the electrons was proposed due the analogy between the Planetary System and the Atom system [4]. The electron moves in an ellipse around the nucleus which is also located in one of the focus of the ellipse [4]. For example, the total energy of a simple harmonic oscillator in one dimension can be described as follows:

$$E = K + V = \frac{p_x^2}{2m} + \frac{1}{2}kx^2 \quad E = \frac{p_x^2}{2m} + \frac{1}{2}kx^2$$

$$1 = \frac{p_x^2}{2mE} + \frac{x^2}{2E/k}$$

Then, the quantization integral of Somerfield can be evaluated by doing a geometrical interpretation [9].

The equation $1 = \frac{p_x^2}{2mE} + \frac{x^2}{2E/k}$ is the equation of an ellipse with coordinates (x, p_x) at the graph p_x versus x .

$$\text{The ellipse equation is as follows: } 1 = \frac{y^2}{b^2} + \frac{x^2}{a^2} \quad b = \sqrt{2mE} \quad \text{and } a = \sqrt{\frac{2E}{k}}$$

$$\oint p_x dx = A \quad \text{where } A \text{ is the area of the ellipse } A = \pi ab$$

$$\oint p_x dx = 2\pi E \sqrt{\frac{m}{k}}$$

The harmonic oscillator as for example a mass on a string [7] has the following equations: $F = -kx = ma$

$$a = -(k/m)x$$

$$a = \frac{d^2x}{dt^2} \quad \frac{d^2x}{dt^2} = -\frac{k}{m}x \quad w^2 = \frac{k}{m} \quad \frac{d^2x}{dt^2} = -w^2x$$

$$\frac{d^2x}{dt^2} + w^2x = 0 \quad x = A\cos(wt + \theta) \quad \frac{dx}{dt} = -Aw\sin(wt + \theta)$$

$$\frac{d^2x}{dt^2} = -Aw^2\cos(wt + \theta) \quad \frac{d^2x}{dt^2} = -w^2x$$

$$-w^2x + w^2x = 0 \quad \text{which satisfies the differential equation}$$

Then, the solution of the harmonic oscillator is $x = A\cos(wt + \theta)$ with angular frequency $w = \sqrt{\frac{k}{m}}$

$$w = 2\pi f$$

$$\oint p_x dx = 2\pi E \sqrt{\frac{m}{k}} = \frac{2\pi E}{w} \quad \oint p_x dx = \frac{2\pi E}{2\pi f} = \frac{E}{f}$$

$$\oint p_x dx = \frac{E}{f} \quad E = nhf : \text{ Planck quantization for the energy of an oscillator [7].}$$

$$\oint p_x dx = n_x h \quad n = 1, 2, 3, \dots$$

The allowed oscillation states are a series of ellipses where h is the distance between two consecutive ellipses. The classic or continuous situation is for $h \approx 0$ or large quantum numbers where all the values of

E are allowed [7]. It is possible to obtain all the quantization rules for the electron at the atom as it was done before: $\oint p_s ds = n_s h$ $s=2\pi r$ $p=mv$

$$mv2\pi r = nh \quad r = \frac{nh}{2\pi mv} \quad m \frac{v^2}{r} = k \frac{e^2}{r^2} \quad \frac{nh}{2\pi mv} = k \frac{e^2}{mv^2} \quad k=1/(4\pi\epsilon_0)$$

$$v = \frac{e^2}{2\epsilon_0 nh} \quad \textbf{Quantization of the velocity}$$

$$r = \frac{\epsilon_0 h^2}{\pi m e^2} n^2 \quad \textbf{Quantization of the radius} \quad a_0 = \frac{\epsilon_0 h^2}{\pi m e^2} \quad \textbf{Bohr Radius}$$

$$E = -\frac{ke^2}{2r} \quad \textbf{Total Bound Energy for the electron at the atom} \quad k=1/(4\pi\epsilon_0)$$

$$E = -\frac{me^4}{8\epsilon_0^2 n^2 h^2} \quad \textbf{Quantization of the energy}$$

$$L=pr \quad L=mv r \quad (\text{constant in a circular motion})$$

$$v = \frac{e^2}{2\epsilon_0 nh} \quad r = \frac{\epsilon_0 n^2 h^2}{\pi m e^2} \quad L = m \frac{e^2}{2\epsilon_0 nh} \frac{\epsilon_0 n^2 h^2}{\pi m e^2}$$

$$L = \frac{nh}{2\pi} \quad \textbf{Quantization of the angular momentum}$$

$$\oint p_s ds = n_s h \quad mv2\pi r = nh \quad pr = n \frac{h}{2\pi} \quad L = \frac{nh}{2\pi}$$

It is possible to obtain the quantization rule for the angular momentum from the Sommerfeld rule as follows: $\oint p_q dq = n_q h$ $p=L$ $q=\theta$ $n_q = l$ (new number).

$$\oint L d\theta = lh \quad \oint d\theta = 2\pi \quad L = l \frac{h}{2\pi}$$

It is in accordance with the Broglie approach that the waves associated with the electron (Schrödinger waves or Pilot waves) must form fixed waves at the stationary states at the atom $2\pi r = n\lambda$ and $\lambda = \frac{h}{mv}$: $mv2\pi r = nh$: $\oint p_s ds = n_s h$. Besides, Bohr condition is the same as the Sommerfeld Condition. Also, De Broglie approach can explain the no emission of radiation at the stationary state and the stability of the atoms [7].

For other hand, the physics variable necessary to determine the form of the electron trajectory is the angular momentum L which has magnitude and direction. The formula of the angular momentum is as follows: $\vec{L} = \vec{r} \times \vec{p}$ $\vec{L} = \vec{r} \times (m\vec{v})$. The direction of the angular momentum is always perpendicular to the trajectory. It is determined by the right hand rule. The magnitude of the angular momentum is given by the next formula: $L = rpsen\theta$ $L = rmvsen\theta$ where θ is the angle between the velocity (v) and the position vector (r). Therefore, if the electron orbit changes of trajectory (r) or changes the velocity (v), then the

magnitude of L also will change. Besides, if the orbit plane changes, the orientation or direction of L will change [4]. Thus, L is a good vector to describe the electron motion.

For other hand, a high relativistic velocity was assigned to the electron in addition to the ellipse motion. It was necessary to apply Relativity Theory to the motion of the electron which experiments mass variation as consequence of the high velocity [4]. As result of this high velocity, all the elliptical orbit has a displacement around the nucleus. It is known as precession which occur also at the Planetary System at the motion of Mercury around the Sun: Perihelium Precession of Mercury [15]. At the Atom System, the electrons moves very close and with high velocities around the nucleus. Then, the relativistic effects are more evident for all the orbits or levels.

In resume, it is necessary to consider two motions for the electron at the atom [4]: the electron trajectory in an ellipse around the nucleus and the displacement of the ellipse around the nucleus or Orbit Precession. Then, the revolution velocity and lineal momentum of the electron at the orbit (determined by the number n) and the angular momentum L and the eccentricity of the ellipse or ellipse precession due the high velocities of the electron which affect the form of the ellipse (determined by the number l) can take only restricted values [14]. Due those restrictions, the electron energy depends of two integer quantum numbers: n and l .

As the angular momentum L describes the form of the displacement of the electron ellipse around the nucleus which considers the orbit precession due the high velocities, the number l makes restrictions to the possible orbits or sub-levels [4]. For a given value of n , l can takes of: $l: 0, 1, 2, 3, \dots, n-1$ $L = l \frac{h}{2\pi}$. Besides, the number l is called by the letters: $s(0), p(1), d(2), f, a, h, i, \dots$. This quantum number is called also azimuthal.

The Somerfield Model was a support for the quantization of the angular momentum and the new quantum sub-level [4]. At the Bohr Model, there are only energy levels n without sub-levels for each energy level. Therefore, when the electron jumps from one orbit to other, there is only emission of one characteristic energy radiation [4]. But at the Somerfield Model, there is some restricted sub-levels l for each energy level n . The sub-levels l within the same level n has energy values very similar. The difference between the Bohr Model and the Somerfield Model is due the magnitude of the angular momentum or the Electron Precession (displacement of the ellipse around the nucleus) which is because of the high relativistic velocity of the electron.

For example, If a sample of any element is excited, then some electrons can get the main level $n=2$. Because there are sub-levels, some electrons arrive to the next sub-levels of the main level $n=2$ $l=0$ $L=0$;

$n=2 \quad l=1 \quad L=\frac{h}{2\pi}$. Then, there is emission of photons due the de-excitation. If the photons does the transition to the energy level $n=1 \quad l=0 \quad L=0$, then the energy of the photons are as follows:

$$E_{21}-E_1=hf_{21}$$

$$E_{20}-E_1=hf_{20}$$

There are two spectral lines very close each other because they have similar energies. This theoretical prediction is in agreement with the experimental results from spectroscopy. If the de-excitation is from the level $n=3$ to the level $n=1 \quad l=0$, then there are more spectral lines due there are more sublevels at the level $n=3$. Nevertheless, Somerfield established that there are forbidden transitions between a sub-level and other level or sublevel. Thus, there are selection rules for the energy jumps between the levels [4]. The values of the quantization of the angular momentum from the Schrödinger Equation is as follows:

$$L = \sqrt{l(l+1)} \frac{h}{2\pi}. \text{ At the Bohr Theory, it is given by: } L=l\frac{h}{2\pi}.$$

For l very large with respect to 1 ($l \gg 1$), the result of the Schrödinger Equation is equal to the result of Bohr Theory for the Hydrogen Atom without sublevels ($L=n\frac{h}{2\pi}$) which is in accordance with the correspondence principle.

m_l : magnetic quantum number which defines the component z (which is the direction of the external magnetic field) of the orbital angular momentum. The component of the orbital angular momentum with respect to the direction of the external magnetic field (L_z) is quantized with this number [4], [5]. It is related with the number and possible spatial orientations of the orbitals and L_z to be occupied by the electron for each value of l due an external magnetic field. This number is product of the interaction of the orbital magnetic dipole momentum of the electron (due the orbital motion of the electron around the nucleus) with the external magnetic field. This number can explain the additional energy sub-levels observed at the Zeeman Effect by the application of an external magnetic field. Those additional energy sub-levels appears only with the application of an external magnetic field. The Zeeman Effect is explained in quantum mechanic at the Schrödinger Theory by considering that the electron have electrical potential energy with the nucleus and potential energy of interaction with an external magnetic field. [4], [5]. Thus, the quantum number m_l appears as result of the external magnetic field. The values of m_l depends of l .

$$L_z = m_l \frac{h}{2\pi} \quad m_l = 0, \pm 1, \pm 2, \dots, \pm l \quad m_l: \text{ magnetic quantum number}$$

In 1896, Zeeman examined what happens to the light emitted by a gaseous sample when the gas is subjected to the action of an intense magnetic field [4]. Zeeman found that the spectral lines appeared

thicker when the atoms were under the action of the magnetic field than when it was not applied [4]. It was found that each spectral line separated into groups of 3 lines. This effect of additional spectral lines by the effect of an external magnetic field was called the Zeeman effect [4], [5]. Those spectral lines are different to the group of lines very near among them due the quantization of the angular momentum and the orbital quantum number without an external magnetic field.

A magnetic field is generated when a wire transports electrical current [4]. Besides, when a wire which transports electrical current is located in an magnetic field perpendicular to the wire, it is generated a magnetic force whose magnitude is: $F = l I B$ (l : length of the wire). Also, if a spire with current I is located in an external magnetic field, it is generated a torque. The effect of this torque or pair of forces is the rotation of the spires [4].

For other hand, at the hydrogen atom, the electron with negative charge rotates around the nucleus with considerable velocity. It is possible to represent the electron as a spires with current I (due the electron). Then, the rotation of the electron generates a small magnetic field [4]. Thus, it is possible to associate to the electron an electric dipole momentum and a magnetic dipole momentum.

Electric Dipole Momentum

If the electric dipole $p = qd$ is located in an electric field $\vec{E}$, the electric dipole changes the direction or orientation to the same direction of the electric field where $F = qE$ [4]. The direction of the dipole charges is possible to know with a test charge with positive sign. The forces of the two charges are in opposite direction. Then, it is generated a torque. The effect of this torque or pair of forces is the rotation of the electric dipole in the clock direction which is the same direction of the electric field[4].

Fig.15. Electric dipole in an electric field

The most stable position for the dipole is when p and E are parallel because the electrical potential energy is minimum $V = -qdE \cos \theta$ (less angle θ or less r): $V = -ke^2/r$. The lines of the electric field starts from the positive charge and finishes at the negative charge. For example, the electric field can be produced by two metallic plaques or capacitors with different charge signs. Therefore, the positive charge has less electrical potential energy: $V = -ke^2/r$ $V = -q d E \cos \theta$ (more negative, less distance between the charge and the plaque or less angle θ), if the positive charge is more close to the negative plaque. At the same way,

a negative charge has less potential energy if the negative charge is more close to the positive plaque [4].

Fig.16. Electric dipole in an electric field generated by two capacitors

Because the distance between the positive charge and the negative charge at the dipole is constant, then the position where the positive charge is more close to the negative plaque and the negative charge is more near to the positive plaque is when E and p are parallel. It is necessary to do a work to change the dipole from the position of minimum energy (E and p parallels) to the position where the dipole has a certain angle with respect to the electrical field. This work is the energy necessary to avoid that the torque (due the external electric field) brings the dipole to the equilibrium position or minimum energy. Thus, an electrical dipole has more energy if it has a certain angle respect to the direction of the field. The potential energy V of the dipole depends of the component of p in the direction of the electrical field E and the magnitude of E :

$$V = -pE \cos\theta \quad p = qd \quad V = -q d E \cos\theta$$

The potential energy is 0 for $\theta = 90^\circ$, $V = -pE$ (minimum energy) for $\theta = 0^\circ$, $V = +pE$ (maximum energy) for $\theta = 180^\circ$. Besides, the dipole has the tendency to be at the position of less energy. It obeys the principle of minimum energy which also correspond to the stationary levels or energies at the atom.

Magnetic Dipole Momentum

A spire with current I has also a magnetic dipole momentum μ . The magnitude of it is as follows: $\mu = IA$ where I is the current that the spires transport and A is the area of the spires. The direction of the vector $\vec{\mu}$ is parallel to the direction of the angular momentum. It is perpendicular to the plane of the spires or the plane of the electron orbit [4].

At the Hydrogen atom, the spires with current are the electron at the atom. At the same way as the electric dipole, a magnetic dipole in a external magnetic field B experiments a torque. The consequence of this torque is that the magnetic dipole u changes the direction or orientation to the same direction of the magnetic field B [4]. As the electric dipole, it is also necessary to do a work to change the magnetic dipole from the position of minimum energy (B and u parallels, $\theta = 0^\circ$) to the position where the magnetic dipole has a certain angle with respect to the magnetic field. This work is the energy necessary to avoid that the torque (due the external magnetic field) brings the magnetic dipole to the equilibrium position.

- As $u=IA$, u changes the value if the current I changes. It is supposed that the area of the spires does not change or changes very little and so, this variation is possible to neglect.
- At the Hydrogen atom, the spires with current is the electron at the atom. The value of I depends of the electron velocity and therefore, it depends of the lineal momentum p .
- The direction of u is given by the direction of the perpendicular to the plane of the electron orbit which is the direction of the angular momentum L .

Therefore, if it is modified the vector $\vec{L}$, then it is also modified the magnitude or direction of $\vec{u}$. In fact, the relation between the angular momentum and the magnetic dipole momentum is as follows: $\vec{u} = -\frac{e}{2m}\vec{L}$ ($\vec{u}$ and $\vec{L}$: antiparallel)

$$L = r p \quad L = r m v \quad \mu = I A = I \pi r^2 = \frac{e}{t} \pi r^2 v = \frac{e}{2} \frac{(2 \pi r)}{t} r^2 = \frac{e}{2} v r$$

$$\frac{\mu}{L} = \frac{e}{2m} \quad \mu = \frac{e}{2m} L$$

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The magnetic dipole momentum u or the angular momentum L associated with the spires (espira) with current which represents the motion of the electron describes a precession motion around the direction of the applied field B (z direction). It is analogous to the motion of the spinning top. When it moves around its axis, it also describes a motion (precession) around of the vertical axis which is the direction of the gravitational force or gravitational field. Besides, it is necessary this rotation in order that it does not go down [4].

An additional potential energy appears due the application of the external magnetic field depending of the orientation or direction of the magnetic dipole momentum μ respect to the magnetic field B [4]:

$$V = -uB \cos\theta \quad V = -u_z B$$

u_z is the component of u in the direction of B which is the z direction.

Then, the total energy of the electron with the application of the external magnetic field is: $E = E_0 + V$

$$V = -u_z B \quad E = E_0 - \mu_z B$$

$$u = -\frac{e}{2m} L \quad \mu_z = -\frac{e}{2m} L_z \quad E = E_0 + \frac{e}{2m} L_z B$$

L_z is the component of L in the direction of B which is the z direction

E_0 : electron energy without the external magnetic field.

E : Total energy of the electron with application of the external magnetic field.

As the angular momentum L is quantized, then the component of L in the z axis (direction of the external magnetic field B), is also quantized:

$$L = \sqrt{l(l+1)} \frac{h}{2\pi} \quad \text{for very large } l: \quad L = l \frac{h}{2\pi} \quad L_z = m_l \frac{h}{2\pi}$$

m_l : magnetic quantum number $m_l = 0, \pm 1, \pm 2, \dots, \pm l$

For example, we have a sample of hydrogen gas where there are many electrons in a excited state with main quantum number $n=2$ and without an external magnetic field. Because, there are sub-levels, some electrons arrive to the next sub-levels of the main level $n=2$:

$$n=2 \quad l=0; n=2 \quad l=1$$

Then, there are emission of photons due the de-excitation. If the photons does the transition to the energy level $n=1 \quad l=0$, then the energy of the photons are as follows: $E_{21}-E_1=hf_{21} \quad E_{20}-E_1=hf_{20}$. There are two spectral lines very close each other because they have similar energies.

There are more spectral lines with the application of the external magnetic field. For example, for the excited state $n=2 \quad l=0$, some electrons only can take angular momentum $L_z=0$ with quantum number

$m_l=0$. As we have mentioned before, for $m_l=0$ (L and B are perpendicular or μ and B are perpendicular), it means that the application of the external magnetic field does not change the total energy of the electron E_0 . For the excited state $n=2$ $l=1$, some electrons can take the states of angular momentum L_z with quantum number $m_l=1$, $m_l=-1$ or $m_l=0$. For $m_l=0$, it means that the application of the external magnetic field does not change the total energy of the electron E_0 and L and B are perpendicular.

The angular momentum L_z and the total energy for each excited level is as follows: $E = E_0 + E_{ml}$

$$E = E_{n,l} + E_{ml}$$

$$L_z = m_l \frac{h}{2\pi} \quad E = E_{n,l} + \frac{e}{2m} L_z B$$

$$l=0,1,2,\dots,n-1 \quad m_l = 0, \pm 1, \pm 2, \dots, \pm l$$

For the initial energy level $n=2$ $l=1$ and $l=0$, the next sub-levels are obtained:

$$n=2 \quad l=1 \quad m_l=1 \quad L_z = \frac{h}{2\pi} \quad E_{2,1,1} = E_{2,1} + \frac{e}{2m} \frac{h}{2\pi} B$$

$$n=2 \quad l=1 \quad m_l=-1 \quad L_z = -\frac{h}{2\pi} \quad E_{2,1,-1} = E_{2,1} - \frac{e}{2m} \frac{h}{2\pi} B$$

$$n=2 \quad l=1 \quad m_l=0 \quad L_z = 0 \quad E_{2,1,0} = E_{2,1}$$

$$n=2 \quad l=0 \quad m_l=0 \quad L_z = 0 \quad E_{2,0,0} = E_{2,0}$$

$E_{2,1}$: energy level with $n=2$, $l=1$ without the external magnetic field.

$E_{2,1,1}$: energy level with $n=2$, $l=1$, $m_l=1$ with the application of the external magnetic field.

Then, at the de-excitation, it is emitted energy radiation with frequency given by the next formula:

$$hf = E_2 - E_1$$

E_1 (stationary state or base level): final energy level of the transition of the electrons from $n=2$ to $n=1$.

The final energy E_1 can take the next sub-levels:

$$n=1 \quad l=0 \quad m_l=0 \quad L_z = 0 \quad E_{1,0,0} = E_{1,0}$$

For the given example (from $n=2$, $l=1$ to $n=1$), the transitions are as follows:

$$hf = E_{2,1,1} - E_{1,0,0}$$

$$hf = E_{2,1,-1} - E_{1,0,0}$$

$$hf = E_{2,1,0} - E_{1,0,0} \quad \text{This line is the same as without external magnetic field.}$$

Therefore, there are new lines (three lines) for the initial level $n=2$, $l=1$ to the final level $n=1$ with the application of the external magnetic field. It is due the interaction between the magnetic dipole

momentum of the electron and the external magnetic field. There is one line more for the level $n=2$ due the next transition: $hf = E_{2,0,0} - E_{1,0,0}$: this line is the same as without external magnetic field. In resume, it appears new group of spectral lines and each group corresponds to one of the spectral lines without the external magnetic field.

For the same sample of hydrogen gas and for the de-excitation with an external magnetic field from the state $n=3, l=2$ to $n=2, l=1$, then there are more spectral lines than before. If the magnetic field is not applied, then it appears only one spectral line: $hf = E_{3,2} - E_{2,1}$. For the excited state $n=3, l=2$ and with the application of the external magnetic field, there are some sub-levels:

$$n=3 \quad l=2 \quad m_l=2 \quad L_z = \frac{2h}{2\pi} \quad E_{3,2,2} = E_{3,2} + \frac{e}{2m} \frac{2h}{2\pi} B$$

$$n=3 \quad l=2 \quad m_l=-2 \quad L_z = \frac{-2h}{2\pi} \quad E_{3,2,-2} = E_{3,2} - \frac{e}{2m} \frac{2h}{2\pi} B$$

$$n=3 \quad l=2 \quad m_l=1 \quad L_z = \frac{h}{2\pi} \quad E_{3,2,1} = E_{3,2} + \frac{e}{2m} \frac{h}{2\pi} B$$

$$n=3 \quad l=2 \quad m_l=-1 \quad L_z = \frac{-h}{2\pi} \quad E_{3,2,-1} = E_{3,2} - \frac{e}{2m} \frac{h}{2\pi} B$$

$$n=3 \quad l=2 \quad m_l=0 \quad L_z = 0 \quad E_{3,2,0} = E_{3,2}$$

$E_{3,2}$: energy level with $n=3, l=2$ without the external magnetic field.

$E_{3,2,2}$: energy level with $n=3, l=2, m_l=2$ with the application of the external magnetic field.

Then at the de-excitation, it is emitted energy radiation with frequency given by the next formula: $hf = E_3 - E_2$ (E_2 (stationary state or base level): it is the final energy level of the transition of the electrons from $n=3$ to $n=2$).

The final energy E_2 ($n=2, l=1$) can take the next sub-levels:

$$n=2 \quad l=1 \quad m_l=1 \quad L_z = \frac{h}{2\pi} \quad E_{2,1,1} = E_{2,1} + \frac{e}{2m} \frac{h}{2\pi} B$$

$$n=2 \quad l=1 \quad m_l=-1 \quad L_z = \frac{-h}{2\pi} \quad E_{2,1,-1} = E_{2,1} - \frac{e}{2m} \frac{h}{2\pi} B$$

$$n=2 \quad l=1 \quad m_l=0 \quad L_z = 0 \quad E_{2,1,0} = E_{2,1}$$

Nevertheless, there are some restriction rules and all the transitions are not allowed. For example, it is not possible the transition from $n=3, l=2, m_l=-2$ to $n=2, l=1, m_l=1$. For the Hydrogen atom, it is possible the transitions with the next rule for the change of l and m_l : $\Delta l = \pm 1$ $l_f - l_i = \pm 1$ and $\Delta m_l = 0, \pm 1$ $m_f - m_i = 0$ or ± 1 where f denotes the final state and i the initial state.

For the given example, the allowed transitions are as follows:

$$hf = E_{3,2,-2} - E_{2,1,-1} \quad hf = E_{3,2,1} - E_{2,1,1} \quad hf = E_{3,2,2} - E_{2,1,1}$$

$$hf = E_{3,2,0} - E_{2,1,1} \quad hf = E_{3,2,0} - E_{2,1,0} \quad hf = E_{3,2,1} - E_{2,1,0}$$

$$hf = E_{3,2,-1} - E_{2,1,0} \quad hf = E_{3,2,-1} - E_{2,1,-1} \quad hf = E_{3,2,0} - E_{2,1,-1}$$

In resume, each spectral line without the magnetic field is divided only in three lines with the application of the external magnetic field by applying the transition rules. These spectral lines have frequencies and energies very similar. If the electron has more number of possible states or levels, the number of the transitions increases and there are more spectral lines [4].

m_s : spin quantum number which defines the component z (which is the direction of the external magnetic field) of the angular momentum of the spin. This number is product of the interaction of the magnetic dipole momentum of spin of the electron (due the spin or model of electron rotation around its own axis) with the external magnetic field. Nevertheless, the spin cannot be understood as a rotated sphere because it is a property with quantum and relativistic origin. Nevertheless, it serves as a model to explain the theory. Besides, the spin cannot be observed experimentally. Only it is possible to mention that the spin is due to an intrinsic motion of the electron [4], [5]. Besides, it is related with the possibility that an orbital occupied by an electron accept or no other electron by applying the Principle of Exclusion of Pauli [8]. In 1925, Wolfgang Pauli discovered a fundamental principle known as Principle of Exclusion of Pauli. This principle has established that two electrons cannot take the same set of quantum numbers: n , l , m_l and m_s . Therefore, these four number cannot be the same for two electrons. Then, two electrons of an atom must have as minimum one different quantum number.

Also, this number can explain the two additional energy sub-levels observed at the Anomalous Zeeman Effect. Those additional energy sub-levels appears only with the application of an external magnetic field [4]. In addition, this number can explain the antiparticles which appear at the Dirac Equation [8].

The Hydrogen Spectrum was successfully explained by introducing the quantization rules for the energy, angular momentum, component z of the angular momentum and with the quantum numbers n , l and m_l . Nevertheless, it was not possible to explain the spectrum for atoms with more than one electron. Thus, it was necessary to introduce a new quantum number m_s and the Principle of Exclusion of Pauli to explain the spectrum of more complex atoms. This quantum number was called spin number [4], [5].

The existence of the spin or the electron rotation around its own axis was demonstrated experimentally by O. Stern and W. Gerlach. In 1925, Goudsmit and Uhlenbeck introduced the hypothesis of the rotation of the electrons around of its own axis as the Planets at the Planetary System. This rotation was called spin. Thus, it was introduced the fourth quantum numbers: the spin number. The electron can be

considered as sphere with a negative charge distributed on its surface uniformly. This representation of the electron as sphere is not real but this model serves to explain the quantization of the magnetic dipole momentum due the spin. Because the electron is a charged particle, this intrinsic motion of the electron generates an additional magnetic dipole momentum due the spin. In 1928, Dirac demonstrated that the angular momentum of the spin is also quantized. It was demonstrated by applying the relativity theory to the quantum theory of the particles as for example to the electron [4], [5].

At the Zeeman Effect, each spectral line is divided into three lines with the application of an external magnetic field. Nevertheless, there are cases with more spectral lines. This effect is known as the Anomalous Zeeman Effect [4] which can be explained by using the spin of the electron. The rotation of the electron on its own axis or spin generated a current I . It is possible to consider the electron as formed by a set of disks located each other together. Each disk has a certain charge on its surface and with the rotation, it is generated a current. Each disk is equivalent to a spire with current [4].

Fig.19. Schematic representation of the spin

Thus, the behaviour of an small magnet and of a spire with current due the influence of an external magnetic field is similar [4]. The direction of the magnetic dipole momentum μ due the spin is from the South to the North by considering the electron as magnet.

Fig.20. Spire with current I and small magnet

As it was mentioned before, a spire with current has a magnetic dipole. A magnetic dipole in an external magnetic field B experiments a torque or pair of forces. The consequence of this torque is that the magnetic dipole changes the direction or orientation at the same direction of the external magnetic field B (minimum energy). It is possible to calculate the magnetic dipole momentum associated with the spin motion of the electron. If the electron is considered as formed by a set of disks located each other together, the magnetic dipole momentum will be the sum of the magnetic momentum due each equivalent

spire or disks. The magnetic dipole momentum due the spin motion is denoted by $\vec{\mu}_s$. As in the orbital motion of the electron, the spin motion has associated the angular momentum to the magnetic dipole momentum.

$$u = -\frac{e}{2m} L \quad \mu_z = -\frac{e}{2m} L_z \quad u_s = -\frac{e}{m} L_s \quad \mu_{sz} = -\frac{e}{m} L_{sz}$$

L_s : spin angular momentum u_s : magnetic dipole momentum of the spin.

$$L_s = pr = I_{\text{Inertia}} \omega \quad I_{\text{Inertia}} = \frac{mr^2}{2} \text{ (Inertia of a cylinder or disk)}$$

$$L_s = \frac{mr^2}{2} \omega = \frac{mr^2}{2} \frac{v}{r} = \frac{mrv}{2} \quad (\omega = v/r)$$

$$u_s = IA = I\pi r^2 = \frac{e}{t} \pi r^2 \quad r = \frac{e(2\pi r)}{t} \quad r = \frac{evr}{2} \quad \frac{\mu_s}{L_s} = \frac{e}{m} \quad u_s = \frac{e}{m} L_s$$

In 1924, O. Stern and W. Gerlach demonstrated experimentally the spin of the electron. The experiment is based in the next fact: the force that experiments a magnetic dipole in presence of a no uniform external magnetic field has a direction and magnitude which depends of the orientation between the dipole and the external magnetic field [4]. The force is variant with different values of magnitude and direction. The field lines generated by an magnet are no uniform. The lines are curves near the North and South Pole. It is possible to observe by using strong filings. Then, the direction and the magnitude of the field is variant.

Fig.21. Field lines generated

It is possible to do an experiment with a large magnet which generates an intense magnetic field (which is analogous to the external magnetic field). Then, the iron filings are directed through the magnet.

Fig.22. Magnet with the field lines and the iron filings directed to the screen

The behaviour of the iron filings are as small dipoles (which are analogous to the electrons) which are deviated of the original trajectory. It is supposed to observe at the screen a continue band blur. It means that the dipoles has experimented different forces. As the forces depend of the orientation between the dipole and the magnetic field, it implies that the dipoles has all the possible orientations. It corresponds a different deviation for each orientation.

At the same way, Stern and Gerlach performed an experiment where a beam of hydrogen atoms were directed through the no uniform external magnetic field. The hydrogen atoms had a particular state: hydrogen atoms with levels $l=0$. Then, the orbital dipole momentum $\mu=0$ $\mu_z=0$ has the value of zero and also the component z (which is the direction of the external magnetic field B) of the angular momentum $L=0$ $L_z=0$ [4].

$$L = \sqrt{l(l+1)} \frac{h}{2\pi} \quad \text{for very large } l, \quad L=l\frac{h}{2\pi}$$

$$l=0 \quad L=0 \quad L_z=0 \quad (L_z \text{ component of } L \text{ in the direction of } B)$$

Besides, if $L=0$, then the orbital magnetic dipole momentum is also zero.

$$\mu = -\frac{e}{2m} L \quad \mu_z = -\frac{e}{2m} L_z \quad \mu=0 \quad \mu_z=0$$

Therefore, if the beam is deviated by the external magnetic field, it proves the existence of an additional magnetic dipole momentum which corresponds to the spin. It is due to the fact that if the hydrogen atoms are only at states with levels $l=0$, then the only interaction with the external magnetic field is only with the magnetic dipole momentum of the spin. Besides, it was observed only two lines very defined at the screen. Therefore, there were only two deviation angles with respect to the incidence direction [4], [5].

The deviation of a beam of dipoles due an external magnetic field depends of the force that experiment the dipole. Besides, the force that experiment a magnetic dipole in an external no uniform magnetic field depends of the relative orientation between the magnetic dipole momentum μ and the external magnetic field B . Therefore, the deviation of the dipoles is influenced by the orientation of the dipoles with the magnetic field [4]. There are three possible options for the dipole deviation:

Parallel Orientation ($\uparrow$): The dipole is deviated to the direction where the magnetic field is more intense (North pole).

Antiparallel Orientation ($\downarrow$): The dipole is deviated to the direction where the magnetic field is less intense (South pole).

Intermediate Orientations: The dipoles have intermediate positions between the parallel and antiparallel orientations.

If the magnetic dipole momentum of the spin have all the possible deviation, then, it will be observed a continue band or blur at the screen as the iron filings. Nevertheless, there were only two lines very defined. It means that the magnetic dipole momentum of the spin only have two orientations respect to the direction of the magnetic field B. In resume, the experiment of Stern and Gerlach demonstrated the spin existence and the two orientations of the spin with respect to an external magnetic field. Then, Goudsmit and Uhlenbeck established the condition that the angular momentum of the spin is quantized. They introduced the quantum number s which is analogous to the number l for the orbital motion or the orbital angular momentum.

$$L_s = \sqrt{s(s+1)} \frac{h}{2\pi} \quad s: \text{spin orbital number for the angular momentum of the spin}$$

Due the experiment of Stern and Gerlach and by theoretical considerations, Goudsmit and Uhlenbeck imposed the condition that the spin orbital number s can take the value of 1/2: $s=1/2$: $L_s = \frac{\sqrt{3}}{2} \frac{h}{2\pi}$

As the orbital magnetic dipole momentum, the interaction between the external magnetic field B and the magnetic dipole momentum of the spin generates an additional energy given by the next formula:

$$V = -u_s B \cos\theta \quad V = -\mu_{sz} B \quad (z \text{ axis: direction of the external magnetic field } B)$$

Then, the total energy of the electron with the application of the external magnetic field is: $E = E_o + V$

$$V = -\mu_{sz} B \quad E = E_o - \mu_{sz} B$$

$$u_s = -\frac{e}{m} L_s \quad \mu_{sz} = -\frac{e}{m} L_{sz} \quad E = E_o + \frac{e}{m} L_{sz} B$$

L_{sz} is the component of L_s (angular momentum of the spin) in the direction of B which is the z direction at this case.

E: electron total energy with the application of the external magnetic field.

E_o : electron energy without the external magnetic field.

As the angular momentum L_s is quantized, then the component of L_s in the z axis (direction of the external magnetic field B), is also quantized by using the quantum number m_s :

$$L_s = \sqrt{s(s+1)} \frac{h}{2\pi} \quad \text{very large } s: L_s = s \frac{h}{2\pi} \quad s = \frac{1}{2} \quad s: \text{spin orbital number}$$

$$L_{sz} = \frac{h}{2\pi} m_s \quad m_s: \text{spin quantum number} \quad m_s = \pm \frac{1}{2}$$

$$L_{sz} = \frac{h}{2\pi} m_s \quad L_{sz} = \pm \frac{1}{2} \frac{h}{2\pi} \quad \mu_{sz} = \pm \frac{1}{2} \left(\frac{eh}{2\pi m} \right)$$

$$E = E_o + \frac{e}{m} L_{sz} B \quad E = E_o \pm \frac{1}{2} \left(\frac{eh}{2\pi m} \right) B$$

Therefore, the additional energy or level which is introduced by the external magnetic field only can take two values: $\pm \frac{1}{2} \left(\frac{eh}{2\pi m} \right) B$. It is also a spatial quantization because the external magnetic field defines a direction for the magnetic dipole momentum of the spin and also two additional energy sub-levels. If the external magnetic field is not applied, then the orientation or direction of the dipoles does not affect the energy levels [4].

In resume, the Anomalous Zeeman Effect and the spin of the electron can explain the additional spectral lines which sometimes appear at the Normal Zeeman Effect. The external magnetic field introduces two additional energy sub-levels to the electron energy: one sub-level due the interaction between the orbital magnetic dipole momentum and the magnetic field and the other sub-level between the magnetic dipole momentum of the spin and the magnetic field. Besides, as the force that experiments the magnetic dipole momentum of the spin depends of the orientation between μ_s and B , if there are only two possible orientations of μ_s , then there are only two values of forces and thus, two deviation angles and two additional energy sub-levels.

4.9. Atoms with more than one electron

Firstly, it is possible to analyze an atom with two electrons. There is an electrostatic interaction between the electron and the other electron in addition to the electrostatic interaction between the electron and the nucleus. It is possible to consider as an approximation that the electron moves in a region where there are the electric field due the nucleus (attractive) and the average electric field due the other electrons (repulsive) [4], [5]. The approximation is because of the mathematic method to solve the Schrödinger Equation but the Schrödinger theory is still valid.

By considering this approximation to the electron motion, it has four quantum numbers: n, l, m_l specifies the orbital motion of the electron (where orbital means a probabilistic region for the electron motion and no circular or elliptical orbit) and m_s specifies the spin orientation. The electrons are in a probabilistic density distribution or region where there are zones for the most probable location of the electron. Those distribution of probabilistic density are called orbitals or electronic clouds. The orbital motion of the electron has energies which depends of the numbers n and l without the external magnetic field. In presence of the external magnetic field, the orbital energy depends also of the quantum number m_l and the total energy depends of m_s in addition.

All the electrons with the same quantum number n are approximately at the same distance to the nucleus. They are at the same orbital or density distribution. The main levels or orbitals are called as follows:

n : 1(K), 2(L), 3(M), 4(N), 5(O), 6(P), 7(Q),....

The probability to find the electron near the nucleus increases when l has a low value. Besides, the energy of the electron decreases when it is more near the nucleus (more negative, less distance r) or l decreases. Then, those electrons with less value of l have less energy for electrons with the same energy level n . For example, electrons with $n=2, l=0$ have less energy than electrons with $n=2, l=1$. The orbital angular momentum is quantized with the quantum number l . It gives an additional energy sub-level for the electron at the atom [4], [5]. The sub-levels l are called as follows:

l : 0(s), 1(p), 2(d), 3(f), 4(g), 5(h), 6(i),.....

The electrons are located in levels and sub-levels at the atom in accordance with the next rules:

- The atoms by means of the electrons try to find an state where the total energy is minimum. It corresponds an state of stability for the atom.
- Two electrons of an atom in a sub-level must have as minimum one different quantum number. It corresponds to the Exclusion Principle of Pauli.

It is possible to apply those rules for the Hydrogen Atom with one electron. The most probable state for the electron is where $n=1, l=0, m_l=0$: $1s^1$. The first number 1 corresponds to the quantum number $n=1$ or level K, the letter s corresponds to the sub-level $l=0$ or s, and the second number 1 corresponds to the number of electrons at the sub-level s or $l=0$. The angular momentum has the value $L=0$ because $l=0$ and $L=l\frac{h}{2\pi}$. We can do the same analysis for the Helium with two electrons. Both electrons have the three first quantum numbers equals but the difference is that one electron takes the quantum number $m_s=1/2$ and the other $m_s=-1/2$: $1s^2$: there are two electrons at the level $n=1$ or K, at the sub-level $l=0$ or s and $m_l=0$ and one electron has $m_s=1/2 \uparrow$ and the other $m_s=-1/2 \downarrow$.

For the sodium with eleven electrons, the configuration is as follows:

First level K: $n=1, l=0, m_l=0, m_s=\pm 1/2$, it can be occupied by two electrons: $1s^2$.

Second level L: $n=2, l=0,1, m_l=0, \pm 1, m_s=\pm 1/2$, the combinations among n, l and m_l are: $n=2, l=0, m_l=0$, $n=2, l=1, m_l=0$, $n=2, l=1, m_l=1$, $n=2, l=1, m_l=-1$.

They can have two combinations more due $m_s=\pm 1/2$. Then, there are 8 possible locations for the electrons at the level L. The formula for the number of possible locations for the electron is $2n^2$. For $n=2$, there are 8 possible locations at this level. For the sodium atom, there are two electrons at the level $n=1$ K, 8 electrons at the level $n=2$ L, and 1 electron at the level $n=3$ M: $\uparrow$. The sodium configuration is as follows: $1s^2, 2s^2, 2p^6, 3s^1$. At the same way, it is possible to obtain the configurations for the periodic table [4], [5]. Nevertheless, there are some variations at the configurations of some elements. These variations starts from the potassium K where the level N starts to fill when the level M is not completely

occupied at all the sub-levels. The electrons support two fields: the field of the nucleus and the field due to the other electrons. The field due the other electrons is more intense when the atomic number is ≥ 19 ($n=19$: K potassium). Therefore, the approximation or model proposed before for the configuration is no so good and it is necessary to do some corrections. Then, it results than the level 4s is of less energy than the level 3d at the Potassium element [4].

The configuration of the electrons is very important for Chemistry where there are relations between the electrons of the external levels and the chemical properties of the elements. Therefore, it has been formed some groups of the elements of the periodic table in accordance with the similar properties among the elements. The elements of the group 1 have one electron at the most external sub-level. Then, they are chemically very active. For other hand, the elements of the group VIII have all the level and sub-levels occupied totally. Then, they don't participate in chemical reactions and they are not chemically active. In resume, the physical and chemical properties of the elements depends of the electronic configurations of the atoms at the base or stationary state and the excited stated [4], [5].

5. Diffraction: Heisenberg's Uncertainty Principle

The Heisenberg uncertainty principle states the following: It is impossible to know simultaneously and exactly the position and moment of a particle. It is expressed with the next formula: $\Delta p \Delta x \geq \frac{h}{2}$ where p is the momentum, x is the position of the particle and h is the Planck constant [4], [5], [9]. A variant of this principle is as follows: It is impossible to know simultaneously and exactly the energy of a particle and the time in which it has that energy:

$\Delta E \Delta t \geq \frac{h}{2}$ where E is the energy and t is the time where this energy is measured. It is demonstrated as follows:

$$E = \frac{p^2}{2m} \quad \Delta E = \frac{2p}{2m} \Delta p \quad \Delta E = v \Delta p$$

$$\Delta x = v \Delta t \quad \Delta t = \frac{\Delta x}{v}$$

$$\Delta E \Delta t = v \Delta p \frac{\Delta x}{v} = \Delta p \Delta x > \frac{h}{2} \quad \Delta E \Delta t \geq \frac{h}{2}$$

This principle is also a support for the modern quantum mechanics and for the Schrödinger's Quantum Theory [4], [5], which is considered as a probabilistic theory. This inability to determine velocity and position exactly and at the same time is not due to an experimental error of the variables or a limitation of the experimental instruments. This impossibility of determination at the same time of these physical variables (velocity and position or energy and time) with all precision is due to an intrinsic property of all

quantum system or of the wave nature of the system due the wave behavior of the electron. In fact, it is possible to obtain the uncertainty principle from the wave properties. Therefore, the quantum nature or wave electron behavior prevents us from determining both variables exactly and at the same time [4], [5], [9]. This is not observed in macroscopic experiments because the quantum scale (microscopic scale) does not take effect and then, it is not observable. Thus, it appears that on a large scale the variables can be accurately determined as the physical instruments allow it.

An imaginary experiment was idealized by Bohr for the Uncertainty Principle. It is possible to measure the position of an electron by means of a microscope. The electron must be illuminated to be observed, since what is observed is not the electron but the scattered photons [9]. At this imaginary experiment, the uncertainty principle appears without doing any calculation or measurement, since the mere fact of observing the electron disturbs it. When the electron is lit, it is bounced by the Compton effect which cannot be determined in detail. But, this is necessary to illuminate the electron to detect it. Thus, the uncertainty principle is inherent in the nature of the quantum processes. There is always an indeterminate interaction between the observer and the observed. The uncertainty principle is a proof of the probabilistic nature of quantum physics [9]. Nevertheless, the electron disturbance can be reduced by using a very weak source. For example, the electron can be illuminated by a single photon entering the microscope lens. The magnitude of the momentum is $p=h/\lambda$. The photon could have been scattered in any direction, within the angle range of 2θ . Thus, the results of the interaction cannot be predicted [9]. The x component of the momentum of the photon can vary from $+p\sin\theta$ to $-p\sin\theta$:

$$\Delta p_x \approx 2p\sin\theta = 2\frac{h}{\lambda}\sin\theta$$

Due to the law of momentum conservation, the electron must receive a momentum in the x direction equal to the change in momentum x of the photon. Then, the momentum of the electron has the same uncertainty of the photon: $\Delta p_x \approx 2\frac{h}{\lambda}\sin\theta$.

It is necessary to use a light with a lower energy, (lower frequency or larger wavelength) or a microscope with a smaller angle θ of measurement (larger D) (which is given by the resolution power of the microscope) to reduce this amount of momentum [9]. The resolution power of the microscope determines the highest precision with which the electron can be located. It is given by the next formula:

$$\sin\theta = 1.28 \frac{\lambda}{D} \quad \sin\theta \approx \frac{\lambda}{D} \quad D \approx \frac{\lambda}{\sin\theta}$$

where D is the linear separation of the points of the object that are solvable in the image: $D=\Delta x$

$$\Delta x = \frac{\lambda}{\sin\theta}$$

Fig.23. Experiment imagined by Bohr for the Uncertainty Principle

The photon is scattered somewhere within the resolvable limits of the microscope. This also corresponds to the uncertainty in the location of the electron $\Delta x = D$. If we want to reduce the localization range Δx , a light with a higher energy, higher frequency or smaller wavelength or a microscope with a higher resolution angle θ should be used (smaller D) [9]. These conditions are contrary to those of momentum. It is a reason that the uncertainty principle appears without doing any calculation or measurement. The

formula is as follows: $\Delta p_x \Delta x = 2 \frac{h}{\lambda} \sin \theta \frac{\lambda}{\sin \theta}$ $\Delta p_x \Delta x = 2h > \frac{(\frac{h}{2\pi})}{2}$

By doing an analysis of the quadratic half values of the respective uncertainties of the position and momentum, it is possible to get the exact formula of the Uncertainty Principle: $\Delta p_x \Delta x > \frac{(\frac{h}{2\pi})}{2}$ Uncertainty Principle of Heissenberg.

Another variant of the experiment is as follows: we want to locate an electron in the vertical position by making it pass through a narrow slit.

Fig.24. Electron diffraction by a slit for the Uncertainty Principle

The figure shows the diffraction spectrum formed on a screen by a beam of monoenergetic electrons passing through a single slit. Due to the particle wave duality, it can be considered as the passage of a flat monochromatic wave with a given wavelength (guide wave or pilot wave) through the slit [5], [9].

Optically, it is known that the first diffraction minimum corresponds to the following formula: $\frac{a}{2} \sin \theta = m \frac{\lambda}{2}$. It is possible to observe at the figure that there is a minimum, if the path difference between the rays that leaves from the superior extreme and from the center is an integer number of the half of the wavelength. The first minimum is obtained when $m=1$: $a \sin \theta = \lambda$ where a is the slit width: $a = \Delta x$ $\sin \theta = \lambda / \Delta x$.

The diffraction spectrum gives the statistical distribution on the screen of a large number of incident electrons from the particle point of view [5], [9]. If $a \gg \lambda$ there is no the diffraction pattern. The diffraction pattern appears when $a \leq \lambda$. If we want to reduce the uncertainty of the y position, it is necessary to reduce the width of the slit (smaller width of the slit) but it increase the diffraction of the electrons and the uncertainty in the momentum. Thus, if we want to reduce the uncertainty in the momentum, it is necessary to increase the the width of the slit. Then, these conditions are contrary to those of the position. The uncertainty principle appears again without doing any calculation or measurement. The uncertainty in the vertical coordinate of the electron is of the order of the width of the slot: $\Delta x \approx a$. The uncertainty in the amount of vertical momentum of the electron Δp_x is given by $\Delta p_x = 2p_x$ (maximum uncertainty of the x component of the momentum: from $-p_x$ to $+p_x$): $\sin \theta \approx \theta = \frac{p_x}{p}$ $p_x = p \sin \theta$

$$p = h / \lambda \quad p_x = \frac{h}{\lambda} \sin \theta$$

$$\Delta p_x = 2p_x \quad \Delta p_x = 2 \frac{h}{\lambda} \sin \theta$$

$$\Delta p_x \Delta x = 2 \frac{h}{\lambda} \sin \theta \Delta x \quad a = \Delta x \quad \sin \theta = \lambda / \Delta x \text{ (first minimum)}$$

$$\Delta p_x \Delta x = 2 \frac{h}{\lambda} \frac{\lambda}{\Delta x} \Delta x \quad \Delta p_x \Delta x = 2h > \frac{(\frac{h}{2\pi})}{2}$$

$$\Delta p_x \Delta x > \frac{(\frac{h}{2\pi})}{2} \quad \text{Uncertainty Principle of Heissenberg}$$

Besides, if the arrival of the electrons are detected with a detector after the slit and before the screen, the behavior of the spectrum at the screen appears as a particle. It is known as the wave collapse. If the total distribution of the electrons is observed on the screen without the detector after the slit, the behavior of the spectrum appears as a wave. It is possible to analyze it with two slits and the result is known as the Copenhagen Interpretation. The probability of an electron hitting some point on the screen is given by the Schröndiger wave function squared [5], [9]. In resume, if we want to reduce the amount of momentum, this increases the uncertainty in the location. On the contrary, if we want to reduce the uncertainty in the location, this increases the uncertainty in the momentum. This imprecision does not depend on the

instruments that are used to measure or the uncertainties of the instruments. This is an inherent property of the quantum nature of physical processes or the wave property of the electron [9].

5.1. Diffraction: Fourier Approach

The constant energy radiation for the case of light before the slit is represented by the next function:

$$f(x,t)=F_0 \quad -x_0/2 \leq x \leq x_0/2$$

$$f(x,t)=0 \quad x > x_0/2 \text{ or } x < -x_0/2$$

Fig.25. Constant energy radiation for the light

The Fourier integral at the domain of the angular frequency w is given by the next function: $F(w) =$

$$F[f(x,t)] = \int_{-\infty}^{\infty} f(x,t) e^{-j\omega t} dt$$

Sometimes, it is considered the Fourier integral function as follows:

$$F(w) = F[f(x,t)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x,t) e^{-j\omega t} dt$$

At this Fourier analysis, it is considered the first function:

$$F(w) = \int_{-x_0/2}^{x_0/2} F_0 e^{-j\omega t} dt$$

$$F(w) = \frac{F_0}{-j\omega} (-2j\omega \frac{wx_0}{2}) \quad e^{-j\omega t} = \cos(\omega t) - j\sin(\omega t)$$

$$F(w) = \frac{2F_0}{\omega} \sin\left(\frac{\omega x_0}{2}\right) = F_0 x_0 \frac{\sin\left(\frac{\omega x_0}{2}\right)}{\frac{\omega x_0}{2}}$$

The magnitude of the spectrum $|F(\omega)|$ para $x_0=2$ and $F_0=7$ is showed in the next figure:

Fig.26. Spectrum $|F(\omega)|$ for the constant radiation for the light

The no constant energy radiation for the case of light or an electromagnetic wave for the case of a beam of electrons before the slit is represented by the next function:

$$f(x,t)=F_0+F_0\cos(w_0t) \quad -x_0/2 \leq x \leq x_0/2 \quad x_0 \leq \lambda_0 \text{ (to produce diffraction)}$$

$$f(x,t)=0 \quad x > x_0/2 \text{ or } x < -x_0/2$$

For $F_0=7$ and $w_0=1$, the graph of $f(x,t)$ is as follows:

Fig.27. No constant energy radiation for a beam of electrons

The Fourier integral at the domain of the angular frequency w is given by the next function:

If $F(w)=F[f(t)]$ the Fourier integral of $f(t)\cos \omega_0 t$ is as follows:

$$F[f(t)e^{j\omega_0 t}] = F(\omega - \omega_0) \quad \cos(\omega_0 t) = \frac{1}{2}[e^{j\omega_0 t} + e^{-j\omega_0 t}]$$

$$\begin{aligned} F[f(t)\cos(\omega_0 t)] &= F\left[f(t)\frac{1}{2}[e^{j\omega_0 t} + e^{-j\omega_0 t}]\right] = \frac{1}{2}F[f(t)e^{j\omega_0 t}] + \frac{1}{2}F[f(t)e^{-j\omega_0 t}] \\ &= \frac{1}{2}F(\omega - \omega_0) + \frac{1}{2}F(\omega + \omega_0) \end{aligned}$$

$$f(x,t)=F_0 \quad -x_0/2 \leq x \leq x_0/2$$

$$f(x,t)=0 \quad x > x_0/2 \text{ or } x < -x_0/2$$

$$F(w) = \frac{2F_0}{w} \text{sen}\left(\frac{wx_0}{2}\right) \quad x_0 \leq \lambda_0$$

$$\frac{1}{2}F(\omega - \omega_0) + \frac{1}{2}F(\omega + \omega_0) = \frac{F_0 \text{sen}\left(\frac{x_0}{2}(\omega - \omega_0)\right)}{\omega - \omega_0} + \frac{F_0 \text{sen}\left(\frac{x_0}{2}(\omega + \omega_0)\right)}{\omega + \omega_0}$$

$$f(x,t)=F_0+F_0\cos(w_0t) \quad -x_0/2 \leq x \leq x_0/2 \quad x_0 \leq \lambda_0 \text{ (to produce diffraction)}$$

$$f(x,t)=0 \quad x > x_0/2 \text{ or } x < -x_0/2$$

$$F(w) = \frac{2F_0}{w} \text{sen}\frac{wx_0}{2} + \frac{F_0 \text{sen}\left(\frac{x_0}{2}(\omega - \omega_0)\right)}{\omega - \omega_0} + \frac{F_0 \text{sen}\left(\frac{x_0}{2}(\omega + \omega_0)\right)}{\omega + \omega_0}$$

$$F(w) = F_0 x_0 \frac{\sin\left(\frac{wx_0}{2}\right)}{\frac{wx_0}{2}} + \frac{F_0 \frac{x_0}{2} \sin\left(\frac{x_0}{2}(w-w_0)\right)}{\frac{x_0}{2}(w-w_0)} + \frac{F_0 \frac{x_0}{2} \sin\left(\frac{x_0}{2}(w+w_0)\right)}{\frac{x_0}{2}(w+w_0)}$$

The magnitude of the spectrum $|F(w)|$ para $x_0=2$, $w_0=0.1$ and $F_0=7$ is showed in the next figure:

Fig.28. Spectrum $|F(w)|$ for a beam of electrons

Therefore, the Fourier Integral represents the intensity of the radiation on the detector screen with angular frequency w $w=2\pi k$ or wave number $k=1/\lambda$. The slit represents a Fourier Integral which gives out the intensity of the radiation. Then, the Fourier Integral of the slit has explained by means of mathematics the Diffraction pattern for the light or for a beam of electrons. Besides, this pattern is explained independently if the incident radiation is considered a beam of wave or particles (light beam or electron beam) [14]. It can explain also the interference pattern for the case of two slits. Because with one slit, the representation of this slit as Fourier Integral works and describes the pattern on the screen, then it must work also for the case of two slits and describes the behavior on the screen for the case of interference [14].

5.2. Uncertainty Principle of Heisenberg by applying Wave Property

In quantum mechanics, the variables E (energy) and t (time) are related and reciprocal quantities which is given by the Uncertainty Principle. Besides, p (momentum) and x or r (position) are also related quantities by the same principle. Besides, the energy is related to the angular frequency $w=2\pi f$ (f : frequency) or $w=2\pi/T$ (T : period) by the formula: $E=\frac{h}{2\pi} w$ $E=\frac{h}{2\pi} 2\pi f$ $E=hf$.

Therefore, other related quantity is the angular frequency w and the time t .

The momentum p is given by the formula: $p=h/\lambda$ and the wave number k is given by the formula $k=2\pi/\lambda$. Then, it is possible to obtain the formula:

$\lambda=2\pi/k$ and $p=\frac{h}{2\pi} k$. Then, other related quantity is the wave number k and the position x or r .

It is possible to analyze the Gaussian Function which appears in many subjects in Physics as in Quantum Mechanics at the harmonic oscillator, Optics, Electronics and for the imagen processing by using filters.

As it has mentioned before, the slit at the diffraction of a beam of electrons or the light represents a Fourier Integral which gives out the intensity of the radiation. Thus, it is possible to obtain the Heisenberg Uncertainty by applying Fourier Integral to the Gaussian Function. In fact, it is possible to obtain the Heisenberg Uncertainty by applying the Fourier Integral independent of the function which is used. The Gaussian Distribution is defined as follows: $f(t) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}}$

It is a function centered in $t=0$ and with rms deviation of $\Delta t_{\text{rms}}=\sigma$. It is possible to calculate the inflexion points as follows:

$$f(t) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}} \quad \frac{df}{dt} = \frac{-t}{\sigma^3\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}}$$

$$\frac{d^2f}{dt^2} = \frac{t^2}{\sigma^5\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}} - \frac{1}{\sigma^3\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}} \quad \frac{t^2}{\sigma^5\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}} - \frac{1}{\sigma^3\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}} = 0$$

$$t^2 = \sigma^2 \quad t = \pm\sigma$$

$$\Delta t_{\text{rms}}=\sigma \quad \text{For } \sigma=2 \quad \Delta t_{\text{rms}}=2$$

Fig.29. Graph of the Gaussian Distribution for $\sigma=2$

In $t=\pm 2$, $f''(t)=0$, then the rms deviation is $\Delta t_{\text{rms}}=2$ which corresponds to the values of t where there are inflexion points. The Fourier Integral of the Gaussian function is obtained as follows:

$$F(w) = F[f(x, t)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x, t) e^{-j\omega t} dt$$

$$F(w) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}} e^{-j\omega t} dt$$

$$F(w) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(t^2 + 2j\sigma^2\omega t)}{2\sigma^2}} dt$$

$$t^2 + 2j\sigma^2\omega t = t^2 + 2j\sigma^2\omega t + (\sigma^2 j\omega)^2 - (\sigma^2 j\omega)^2$$

$$t^2 + 2j\sigma^2\omega t = (t + j\sigma^2\omega)^2 - (\sigma^2 j\omega)^2$$

$$F(w) = \frac{e^{-\frac{\sigma^2\omega^2}{2}}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(t+j\sigma^2\omega)^2}{2\sigma^2}} dt$$

$$x = \frac{(t+j\sigma^2 w)^2}{2\sigma^2} \quad dt = \sqrt{2}\sigma dx$$

$$F(w) = \frac{e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{\sigma\sqrt{2\pi}} e^{-x^2} \sqrt{2}\sigma dx$$

$$F(w) = \frac{e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi}} e^{-x^2} dx$$

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi}} e^{-x^2} dx = 1$$

$$F(w) = \frac{e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}}$$

This function is also Gaussian centered in $w=0$ and with rms deviation of $\Delta w_{\text{rms}}=1/\sigma$. It is possible to calculate the inflexion points as follows:

$$F(w) = \frac{e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} \quad \frac{dF}{dw} = -\frac{\sigma^2 w e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}}$$

$$\frac{d^2 F}{dw^2} = \frac{\sigma^4 w^2 e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} - \frac{\sigma^2 e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} \quad \frac{\sigma^4 w^2 e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} - \frac{\sigma^2 e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} = 0$$

$$\sigma^4 w^2 = \sigma^2$$

$$w^2 = \frac{1}{\sigma^2} \quad w = \pm \frac{1}{\sigma}$$

$$\Delta w_{\text{rms}} = \frac{1}{\sigma} \quad \text{For } \sigma=2 \quad \Delta w_{\text{rms}}=1/2$$

Fig.30. Graph of the Fourier Integral of the Gaussian Distribution for $\sigma=2$

In $w=\pm 0.5$, $F''(w)=0$, then the rms deviation $\Delta w_{\text{rms}}=0.5$ which corresponds to the values of w where there are inflexion points. Therefore, it is obtained for the related quantities: $\Delta w \Delta t = \frac{1}{\sigma} \sigma = 1$ for a gaussian distribution. For the Gaussian function, this product is one independent of the value of σ .

In Physic terms, it means that if the time is increased or stretched (more Δt), then it implies a decrease or narrowed (less Δw) at the frequency spectrum (more waves). It is possible to appreciate this inverse

relation between time and frequency in Electronics by using an oscilloscope. For the other related quantities, it is obtained the same relation: $\Delta k \Delta x = 1$: gaussian distribution.

If the position is increased or stretched (more Δx), then it implies a decrease or narrowed (less Δk) at the wave-number spectrum (more waves). Those relations are applied in quantum mechanics by introducing the formula for momentum and energy given by De Broglie and Einstein:

$$E = hf \quad w = 2\pi f \quad f = w/(2\pi) \quad E = \frac{h}{2\pi} w$$

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

The formula are as follows:

$$\Delta w \Delta t = 1 \quad E = \frac{h}{2\pi} w \quad \frac{h}{2\pi} \Delta w \Delta t = \frac{h}{2\pi} \quad \Delta E \Delta t = \frac{h}{2\pi}$$

$$\Delta k \Delta x = 1 \quad p = \frac{h}{2\pi} k \quad \frac{h}{2\pi} \Delta k \Delta x = \frac{h}{2\pi} \quad \Delta p \Delta x = \frac{h}{2\pi}$$

Nevertheless, $f(t)$ represents a wave function with no physical interpretation. The wave function squared is the quantity that has direct physical significance and it is the one that is related to the experimental results. The squared function $|f(t)|^2$ is known as the probability amplitude which is also a Gaussian function. The probability amplitude in the frequency is $|f(w)|^2$ which is also Gaussian function. The rms deviation of $|f(t)|^2$ is $\frac{\sigma}{\sqrt{2}}$ and the rms deviation of $|f(w)|^2$ is $\frac{1}{\sigma\sqrt{2}}$.

$$f(t) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}} \quad |f(t)|^2 = g(t) = \frac{1}{\sigma^2 2\pi} e^{-\frac{t^2}{\sigma^2}}$$

$$\frac{dg}{dt} = \frac{-2t}{\sigma^4 2\pi} e^{-\frac{t^2}{\sigma^2}} \quad \frac{d^2 g}{dt^2} = \frac{4t^2}{\sigma^6 2\pi} e^{-\frac{t^2}{\sigma^2}} - \frac{2}{\sigma^4 2\pi} e^{-\frac{t^2}{\sigma^2}}$$

$$t^2 = \frac{\sigma^2}{2} \quad t = \pm \frac{\sigma}{\sqrt{2}} \quad \Delta t_{\text{rms}} = \frac{\sigma}{\sqrt{2}}$$

By doing the same procedure, it is possible to obtain $\Delta w_{\text{rms}} = \frac{1}{\sigma\sqrt{2}}$ for $|f(w)|^2$.

$$F(w) = \frac{e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} \quad |F(w)|^2 = h(w) = \frac{1}{2\pi} e^{-\sigma^2 w^2}$$

$$\frac{dh}{dw} = -\frac{2\sigma^2 w e^{-\sigma^2 w^2}}{2\pi} \quad \frac{d^2 h}{dw^2} = \frac{4\sigma^4 w^2 e^{-\sigma^2 w^2}}{2\pi} - \frac{2\sigma^2 e^{-\sigma^2 w^2}}{2\pi}$$

$$\frac{4\sigma^4 w^2 e^{-\sigma^2 w^2}}{2\pi} - \frac{2\sigma^2 e^{-\sigma^2 w^2}}{2\pi} = 0$$

$$4\sigma^4 w^2 = 2\sigma^2 \quad w^2 = \frac{1}{2\sigma^2}$$

$$w = \pm \frac{1}{\sqrt{2}\sigma} \quad \Delta w_{\text{rms}} = \frac{1}{\sigma\sqrt{2}}$$

Therefore, the formula of the Uncertainty Principle is as follows:

$$\Delta w \Delta t = \frac{1}{\sigma\sqrt{2}} \frac{\sigma}{\sqrt{2}} = \frac{1}{2}$$

$$\Delta k \Delta x = \frac{1}{\sigma\sqrt{2}} \frac{\sigma}{\sqrt{2}} = \frac{1}{2}$$

$$\Delta w \Delta t = \frac{1}{2} \quad E = \frac{h}{2\pi} w \quad \frac{h}{2\pi} \Delta w \Delta t = \frac{\frac{h}{2\pi}}{2} \quad \Delta E \Delta t = \frac{\frac{h}{2\pi}}{2}$$

$$\Delta k \Delta x = \frac{1}{2} \quad p = \frac{h}{2\pi} k \quad \frac{h}{2\pi} \Delta k \Delta x = \frac{\frac{h}{2\pi}}{2} \quad \Delta p \Delta x = \frac{\frac{h}{2\pi}}{2}$$

The factor 1/2 appears because it is using Gaussian distribution for the wave function $f(t)$. Nevertheless, it is obtained a factor of: $c \frac{h}{2\pi}$ for the product of $\Delta E \Delta t$ or $\Delta p \Delta x$ independent of which function is used.

$$\Delta E \Delta t = c \frac{h}{2\pi} \quad \text{or} \quad \Delta p \Delta x = c \frac{h}{2\pi} \quad \text{for any function where } c \text{ is a constant}$$

The factor 1/2 due the Gaussian function is the minimum possible for the factor $\Delta E \Delta t$ or $\Delta p \Delta x$: $c \geq 1/2$. The Gaussian Distribution is called the minimum packet of dispersion. Therefore, the Uncertainty Principle of Heisenberg is as follows:

$$\Delta E \Delta t \geq \frac{\frac{h}{2\pi}}{2} \quad \Delta p \Delta x \geq \frac{\frac{h}{2\pi}}{2}$$

6. Interference: Double Slit Experiment

A beam of electrons is fired at two parallel slits. They are detected on a screen which is the detector of the interference pattern. The electron beam will create a pattern of light and dark bands if there is no other detector after the slit and before the screen. This pattern behavior is similar to the waves pattern which is a proof of the duality wave-particle of De Broglie. It is also a proof of the standing waves for the electron to explain the stationary states at the atom by applying the De Broglie Approach [9].

Fig.31. Double Slit Experiment with the intensity pattern on the screen detector

But, if an observer put a detector after the slit and before the screen to know which slit each electron passes, only two bright spots will appear and the interference pattern disappears. It is as if the electrons were bullets fired through one slit or the other. This pattern behavior is equal to the particle behaviour. It is known as the collapse of the wave pattern (wave collapse) and one explanation was the Copenhagen Interpretation.

If φ_A and φ_B (wave functions for each slit) are different wave function for the electron. They are solutions of the Schrödinger Equation. Besides, they represent a possible state for the electron [5]. Then, the superposition of the two waves is also solution of the Schrödinger equation: $\varphi = c_1 \varphi_A + c_2 \varphi_B$ where c_1 and c_2 are constants. The electrons at the two slits experiment have the same probability to pass in each slit. The interference pattern observed for the electron is the same as the light interference. It is possible to understand by applying the wave-particle duality of De Broglie. If it is not located a detector before the screen and after the slit, it is not possible to know which slit the electron has passed. The electron is in a superposition of states given by the next function: $\varphi = \frac{1}{\sqrt{2}}(\varphi_A + \varphi_B)$. The coefficient $\frac{1}{\sqrt{2}}$ is due that the electron has the same probability to pass in the slit A or B. It is possible to obtain this number by the condition that the probability of that the electron in some region of the element volume is the unity:

$\int |\varphi|^2 dV = 1$ Because φ is a probabilistic wave function

The distribution of the electrons at the screen is given as follows:

$$\begin{aligned} |\varphi|^2 &= \varphi * \varphi^* = \frac{1}{\sqrt{2}}(\varphi_A + \varphi_B) \frac{1}{\sqrt{2}}(\varphi_A^* + \varphi_B^*) \\ &= \frac{1}{2}(|\varphi_A|^2 + |\varphi_B|^2 + \varphi_A \varphi_B^* + \varphi_A^* \varphi_B) \end{aligned}$$

Therefore, the term $\varphi_A \varphi_B^* + \varphi_A^* \varphi_B$ contributes to the respective pattern on the screen and makes the difference with the particle pattern on the screen which does not include this term. This pattern is similar to the light interference pattern. It is in agreement with the consideration for the electron as wave. It is obtained the same pattern independent if millions of electrons arrive by second, or only one electron by hour. Of course, it is needed many electrons to obtain the interference pattern as the light interference [5]. It is similar to the throwing of a coin where it is necessary to do many throwing of the coin to prove the probability of 1/2 for each side of the coin. This uncertainty principle also is a support for the probabilistic model of the Schrödinger Approach. Besides, this probabilistic behaviour is used at the Schrödinger Theory which is a Probabilistic Theory for the electron at the atom.

For the light case, the interference is product of the interference of the two light waves when they pass through the slits. For the electron case, it is possible to consider the electron as wave and therefore, it is obtained the same result as the light because of the interference of two electron waves from the two slits.

As we mentioned before, it is necessary many electrons to observe the pattern because of the probabilistic behavior. One electron only produces a point at the screen and with few electrons the pattern is not good observable. The electrons during the wave interference are located in different positions at the total wave $\varphi = c_1 \varphi_A + c_2 \varphi_B$ but that we observe on the screen is the total interference wave φ . The wave serves to the electron as guide during the interference process. The electrons from the wave φ_A or φ_B after the slits are positioned in a new guide wave φ whose pattern is observed at the screen. The explanation for the interference pattern was explained with two proposed: The Copenhagen Interpretation and the Pilot Wave Interpretation.

6.1. The Copenhagen Interpretation

The modern quantum mechanics has established that the electrons do not have definite positions. The electrons spread out like a wave with no definite position which is a probabilistic solution of the Schrödinger Equation [4], [5]. Thus, it is necessary to consider probabilistic approach to calculate the probabilistic position of the electron. At the double slit experiment, the electron passes through both slits simultaneously, and interferes with itself to form the bright and dark bands on the screen [5]. If the observer put a detector before the screen to know which slit each electron passes, only two bright spots will appear and the interference pattern disappears. The observation by using the detector collapses instantaneously the wave interference pattern.

6.2. Pilot Wave Interpretation and why the electron doesn't radiate energy as a particle

This interpretation was proposed by Bohmian. It is a new interpretation of quantum mechanics. At this interpretation, the electrons are guided by a pilot wave like a surfer on a wave. Every electron always has a definite position like the surfer because the electron is a particle guided by a wave. It doesn't matter if the observer knows the position or not. An electron is pushed or guided by a guiding pilot wave which influences the electron's location. The interference spectrum gives the statistical distribution on the screen of a large number of incident electrons from the particle point of view. From the wave point of view, the interference of the pilot waves gives out the interference pattern. The wave serves to the electron as guide during the interference process. Each electron travels through one slit or the other, but the pilot wave passes through both slits simultaneously. The electrons from the wave φ_A or φ_B after the slits are positioned in a new guide wave φ whose pattern is observed at the screen. A measurement or observation at the slits will collapse the pilot wave and detect the electron position at this point.

The electron doesn't radiate energy as a particle because the electron in an atom no excited is at rest. Thus, it cannot radiate energy because it corresponds to a stationary level of the atom. Besides, the electron is guided by a pilot wave and it is a rest within the wave. It is similar for an astronaut inside of a

rocket which is moving with a constant velocity v . Then, the astronaut is at rest within the rocket. In similar form, the electron is at rest within the wave and therefore, the electron does not radiate energy.

7. Heisenberg Approach: Matrix Approach

Heisenberg proposed a matrix mechanic. This is a theory that makes application of observable quantities. By means of Bohr's correspondence principle, the stationary states of the atom were obtained. Heisenberg applied Fourier analysis and Hamiltonian Concept to the quantum world. Balmer's formula depended on two index n and n' . He postulated that there should be as many indices as stationary states. Heisenberg affirmed that all classical physical magnitude must be transformed into a matrix A_{nm} . The position of the electron x must be replaced by a matrix X_{nm} [4], [5], [8]. The matrix development for the position of the electron is: $x_{nm}^2 = \sum_k x_{nk} x_{km}$. The Dynamics that govern quantum quantities is as follows:

$$\frac{dX}{dt} = \frac{i}{\hbar} (HX - XH) = \frac{i}{\hbar} [H, X] \text{ where } H \text{ is the hamiltonian matrix or the energy.}$$

$[H, H] = 0$ which represents the conservation of energy.

Through the application of the Hamiltonian and the matrix application, Heisenberg was able to obtain the energy conservation. The Heisenberg matrix mechanics was developed by Heisenberg, Born and Jordan. It explained very well the observations and experimental results [4], [5], [8]. In addition, Heisenberg discovered a principle known as the Uncertainty Principle: the impossibility of knowing at the same time and with all precision the position and velocity (or momentum) of an electron or the energy and the instant at which it is measured [4], [5], [8], [9]: $\Delta E \Delta t \geq \frac{\hbar}{2}$ $\Delta p \Delta x \geq \frac{\hbar}{2}$.

The electron is never found between the stationary states in the Heisenberg model. The electron does not have this property. Thus, in the game of chess, the only interest is the initial position of a pawn and its final position and it does not matter how the pawn's trajectory was. It is the same as in Heisenberg's matrix theory. In the matrix theory developed by Heisenberg: the motion of the electron within the atom is not the translation of the electron ball in some path around the nucleus. The movement of the electron within the atom is the change of the state of the system in the time that is described by means of the matrix where it is only matter the initial position and the final position. The problem of the stability of the atom was solved because in an unexcited atom, the electron is at rest and therefore should not radiate.

This corresponds to a state at rest and to a stationary matrix solution. The atom in this matrix model was presented as an infinite chess board where in each square was written the numbers of the matrices X_{nk} (n : abscissa and k : ordered). These numbers were the coordinates of the electron in the atom [4], [5], [8].

This matrix development was not widely accepted by scientists of that time. Schrodinger's wave mechanics received more acceptance among physicists.

8. Schrödinger Quantum Theory

The modern quantum physics describes the behavior of atoms and matter in the microscopic system without mixing the classical and quantum concept. This quantum development was carried out by Schrödinger, Heisenberg, Born, De Broglie and Dirac. This explained almost all the experimental evidences at the atom [4], [5].

The ideas established before the modern quantum physics are still valid as for example: the quantization of the energy and the Planck constant, the quantization of the angular momentum, wave properties of the matter, particle properties of the radiation, wave-particle duality, Heisenberg Uncertainty Principle and the Probabilistic Interpretation for one slit and two slits for the diffraction and interference, [9]. The fundamental principles of modern quantum mechanics are: Heisenberg's uncertainty principle and de Broglie's wave-particle duality behavior of matter. De Broglie wave-particle duality was used by Schrödinger to create his quantum theory by means of the wave equation and the wave function associated with the particle [4], [5].

In 1926, Schrödinger used the investigation of De Broglie applied with the Hamiltonian Approach and obtained an equation (wave equation) in which electrons are represented by means of waves [4], [5]. This was the beginning of modern quantum mechanics [4], [5]. The Schrödinger wave equation applied at the atom at the microscopic scale is analogous to Newton's second law: $F = ma$ $F = m \frac{dv}{dt}$ applied at the macroscopic scale. By solving Newton's second law, all the characteristics of the particle, trajectory and velocity are obtained in a deterministic behaviour. Likewise, when the Schrödinger equation is solved, the wave function associated with the electron or object of study is obtained. Furthermore, the wave function contains information about the energy of the particle and its momentum. But, momentum and energy cannot be interpreted classically. These quantities have a probabilistic interpretation and no deterministic. In this way, all the dynamic quantities obtained from the electron have a probabilistic interpretation at the Schrödinger Theory. Those Dynamic quantities are obtained by solving the Schrödinger Equation by using the squared wave function.

Therefore, the motion of the electron at the atom can be described by the electron wave (probabilistic wave) which satisfies the Schrödinger Equation at the stationary energy levels. As it was mentioned before, the information of this wave function is probabilistic with no physical interpretation and no deterministic as the solution of the Newton equation. The wave function acts as an intermediary between the wave equation and its squared function which has physical significance and it is the one that is related

to the experimental results [4], [5]. The squared function is known as the probability amplitude. The wave function squared gives us the probability of finding the electron within a given volume with a given quantized energy. The electron is located in a probabilistic region called orbital [4], [5]. Thus, the square of the wave function evaluated at a given point in space and at a defined time, gives us the probability of finding the particle at that point and at that specific instant [4], [5].

Also, the modern quantum physics could explain the postulates of Bohr and obtain the quantization formula for the energy and angular momentum at the stationary levels by applying the Schrödinger (wave probabilistic theory) and Heisenberg Theory (matrix theory) [4], [5]. The stationary states or levels correspond to those functions which satisfy the Schrödinger Equation [4], [5].

It is similar to the conditions of normal modes for a wave as at the harmonic oscillator. The electron in an atom not excited is at rest. Thus, it cannot radiate energy because it corresponds to a stationary level of the atom [4], [5]. The quantum numbers n (main number), l (orbital number), m_l (magnetic number) and m_s (spin number) are obtained directly from the Schrödinger Equation. It is not necessary to apply some postulates as the Bohr Theory [4], [5]. The Schrödinger theory is stronger than the Bohr theory in the sense that it is not necessary to use postulated ad hoc or patches to explain the results. Also, the Schrödinger Theory doesn't use classic concepts. The Schrödinger Equation is not possible to derive mathematically. It was an imposed postulate as the Second Newton Formula.

The Schrödinger Equation dependent of the time is as follows:

$$-\frac{\left(\frac{h}{2\pi}\right)^2}{2m} \frac{\partial^2}{\partial x^2} \varphi + V(x)\varphi = i \frac{h}{2\pi} \frac{\partial \varphi}{\partial t} \quad \mathbf{1D}$$

$$-\frac{\left(\frac{h}{2\pi}\right)^2}{2m} \left(\frac{\partial^2}{\partial x^2} \varphi + \frac{\partial^2}{\partial y^2} \varphi + \frac{\partial^2}{\partial z^2} \varphi \right) + V(x)\varphi = i \frac{h}{2\pi} \frac{\partial \varphi}{\partial t} \quad \mathbf{3D}$$

The Schrödinger Equation independent of the time is as follows:

$$-\frac{\left(\frac{h}{2\pi}\right)^2}{2m} \frac{\partial^2}{\partial x^2} \varphi + V(x)\varphi = E\varphi \quad \mathbf{1D}$$

$$-\frac{\left(\frac{h}{2\pi}\right)^2}{2m} \left(\frac{\partial^2}{\partial x^2} \varphi + \frac{\partial^2}{\partial y^2} \varphi + \frac{\partial^2}{\partial z^2} \varphi \right) + V(x)\varphi = E\varphi \quad \mathbf{3D}$$

$\int |\varphi|^2 dV = 1$ because φ is a probabilistic wave function

For a free particle, the potential has the value of 0, $V=0$.

The solution of the Schrödinger equation for a free electron ($V=0$) with motion between $-L/2$ and $L/2$, and with even parity symmetry is:

$$\varphi(x,t) = A \cos(kx + \omega t) \quad k = 2\pi/\lambda$$

$$-\frac{\left(\frac{h}{2\pi}\right)^2}{2m} \frac{\partial^2}{\partial x^2} \varphi + V(x)\varphi = E\varphi \quad V=0$$

$$-\frac{\left(\frac{h}{2\pi}\right)^2}{2m} (-Ak^2) = EA \quad E = \frac{\left(\frac{h}{2\pi}\right)^2}{2m} k^2 \quad k = 2\pi/\lambda$$

$$E = \frac{h^2}{2m\lambda^2} \quad V=0 \quad E=K \quad K = \frac{1}{2}mv^2 \quad K = \frac{p^2}{2m}$$

$$\frac{h^2}{2m\lambda^2} = \frac{p^2}{2m} \quad p = \frac{h}{\lambda}$$

It is the formula of De Broglie for the wave-particle duality. It is a strong proof for the validity of the Schrödinger Equation.

For $t=0$, the function must be zero in $x=\pm L/2$ and $x>L/2 \quad \varphi=0 \quad x<-L/2 \quad \varphi=0$

$$\cos(kL/2)=0 \quad kL/2=(2n-1)\pi/2 \quad kL=(2n-1)\pi \quad n=1,2,3,\dots$$

For $n=0$, it is the trivial solution $\varphi=0$. The solution for the energy is as follows:

$$E = \frac{\left(\frac{h}{2\pi}\right)^2}{2m} k^2 \quad E = \frac{\left(\frac{h}{2\pi}\right)^2}{2m} \left(\frac{2\pi}{L}\right)^2 \left(n - \frac{1}{2}\right)^2 \quad n=1,2,3,\dots$$

If we consider the free electron ($V=0$) with motion between $-L/2$ and $L/2$, other possible solution is $\varphi = A \sin(kx + \omega t)$ which has odd parity symmetry [5].

$$E = \frac{\left(\frac{h}{2\pi}\right)^2}{2m} k^2 \quad E = \frac{h^2}{2m\lambda^2} \quad x>L/2 \quad \varphi=0 \quad x<-L/2 \quad \varphi=0$$

For $t=0$, the function must be zero in $x=\pm L/2$

$$\sin(kL/2)=0 \quad kL/2=n\pi \quad n=1,2,3,\dots$$

For $n=0$, it is the trivial solution $\varphi=0$. The solution for the energy is as follows:

$$E = \frac{\left(\frac{h}{2\pi}\right)^2}{2m} k^2 \quad E = \frac{\left(\frac{h}{2\pi}\right)^2}{2m} \left(\frac{2\pi}{L}\right)^2 n^2$$

In resumen, it is obtained discrete values of energy for the free electron located between $-L/2 < x < L/2$. The electron can not be in any of these states of energy. The general solution is a superposition of energy states [5]: $\varphi = \sum C_E \varphi_E$

Where, C_E is the probability to find the electron in the energy state E [5].

The energies of the electrons will be distributed with the probabilistic amount C_E^2 .

Hydrogen Atom

The results from the Schrödinger Equation for the Hydrogen Atom are in concordance with the evidences and experimental results as the Normal Zeeman Effect, Anomale Zeeman Effect, Spectrum of Fine Structure for example [4], [5]. The Schrödinger Equation for the Hydrogen Atom is very similar to other atoms with one electron or Hydrogenids as Ionized Helium. This approach is possible to apply to all those atoms with one electron but the Schrödinger equation is possible to apply for any configuration or electron number of the atom.

For the Hydrogen Atom, it is necessary to know the potential energy. The solution of the radial equation depends of the potential energy function:

$$V(r) = -k \frac{Ze^2}{r} \quad r = \sqrt{x^2 + y^2 + z^2}$$

Ze: electric charge of the nucleus $k=1/(4\pi\epsilon_0)$

It is possible to use the reduced mass: $\mu = m(\frac{M}{m+M})$

$$-\left(\frac{h}{2\pi}\right)^2 \left(\frac{\partial^2}{\partial x^2} \varphi + \frac{\partial^2}{\partial y^2} \varphi + \frac{\partial^2}{\partial z^2} \varphi \right) - k \frac{Ze^2}{r} \varphi = E\varphi$$

By solving this equation in spherical coordinates, it is possible to obtain the radial form of the equation [16]:

$$-\left(\frac{h}{2\pi}\right)^2 \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) - \frac{\left(\frac{h}{2\pi}\right)^2}{2\mu r^2} \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2 \psi}{\partial \Phi^2} \right] \right] + V(r)\psi = E\psi$$

where the general solution is $\psi(r, \theta, \Phi) = R(r)f(\theta)g(\Phi) = R(r)Y(\theta, \Phi)$

$$L_{op}^2 = -\left(\frac{h}{2\pi}\right)^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \Phi^2} \right]$$

$$-\left(\frac{h}{2\pi}\right)^2 \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) \right] + \frac{L_{op}^2}{2\mu r^2} \psi + V(r)\psi = E\psi \quad \psi(r, \theta, \Phi) = R(r)Y(\theta, \Phi)$$

$$-\frac{\left(\frac{h}{2\pi}\right)^2}{2\mu r^2} Y(\theta, \Phi) \frac{d(r^2 R')}{dr} + \frac{R}{2\mu r^2} L_{op}^2 Y(\theta, \Phi) + V(r)R(r)Y(\theta, \Phi) = ER(r)Y(\theta, \Phi)$$

By dividing for $R(r)Y(\theta, \Phi)$, it is obtained:

$$\frac{1}{\left(\frac{h}{2\pi}\right)^2 Y(\theta, \Phi)} L_{op}^2 Y(\theta, \Phi) = \frac{2\mu r^2}{\left(\frac{h}{2\pi}\right)^2} [E - V(r)] + \frac{1}{R} \frac{d(r^2 R')}{dr}$$

Each side of the equation must be equal to a constant α because the left side depends of θ and Φ and the right side depends of r .

$$L_{op}^2 Y(\theta, \Phi) = \alpha \left(\frac{h}{2\pi}\right)^2 Y(\theta, \Phi)$$

This is the equation for eigenvalues for L_{op}^2 . There is the solution only for certain values of α . Then the square of the angular momentum is quantized. The values of α which are solutions for the L_{op}^2 are: 0,2,6,12,...

$$\alpha = l(l+1) \quad l=0,1,2,3,\dots$$

$$L = \sqrt{l(l+1)} \frac{h}{2\pi}$$

$$Y_{lm}(\theta, \Phi) = e^{im\Phi} f_{|m|}(\theta) \quad f_{|m|}(\theta) : \text{function of Legendre}$$

$$m=m_l \quad m=0, \pm 1, \pm 2, \dots, \pm l$$

$$-\frac{\left(\frac{h}{2\pi}\right)^2}{2\mu r^2} \frac{d(r^2 R')}{dr} + \left[\frac{\alpha \left(\frac{h}{2\pi}\right)^2}{2\mu r^2} + V(r) \right] R = ER$$

This is the radial equation. It is possible to replace the value of α and the potential function at the radial equation and it is obtained:

$$-\frac{\left(\frac{h}{2\pi}\right)^2}{2\mu r^2} \frac{d(r^2 R')}{dr} + \left[\frac{l(l+1)\left(\frac{h}{2\pi}\right)^2}{2\mu r^2} - k \frac{Ze^2}{r} \right] R = ER$$

If the total energy is positive the electron is not bounded to the atom. Then, we consider only negative energy with $V(r) > E$ for high values of r . There are solutions with good behavior only for certain values of E . For other values of E , R has the tendency to ∞ for high values of r [16]. The solution is as follows: $\psi(r, \theta, \Phi) = R(r)f(\theta)g(\Phi) = R(r)Y_{lm}(\theta, \Phi)$.

It is possible to consider the solution for the lower energy at the base level: $l=0$. It is the value of l for the lower angular momentum and kinetic energy [16]. It is possible the parameter λ in the next form because of the negative energy: $\lambda^2 = -\frac{2\mu E}{\left(\frac{h}{2\pi}\right)^2}$.

$$\frac{1}{r^2} \frac{d(r^2 R')}{dr} + \frac{2\mu k Ze^2}{\left(\frac{h}{2\pi}\right)^2} \frac{R}{r} = \lambda^2 R$$

$$R'' + \left(\frac{2R'}{r} + \frac{2\mu k Ze^2}{\left(\frac{h}{2\pi}\right)^2} \frac{R}{r} \right) = \lambda^2 R$$

The solution must have the tendency to zero when r has the tendency to ∞ . For r with very high value, the term in parenthesis has very low value and the equation can be written in the next form: $R'' \approx \lambda^2 R$.

The functions $e^{-\lambda r}$ and $e^{+\lambda r}$ satisfies the equation. If λ is positive, $e^{+\lambda r}$ is ∞ for high values of r . Then, for high values of r , the solution is $e^{-\lambda r}$.

$$R \approx e^{-\lambda r}$$

It is the solution for all values of r if the term in parenthesis at the equation has the zero value. It occurs for a particular value of λ .

$$R' = -\lambda e^{-\lambda r} = -\lambda R$$

$$-\frac{2\lambda R}{r} + \frac{2\mu kZe^2}{\left(\frac{h}{2\pi}\right)^2} \frac{R}{r} = 0$$

$$\lambda = \frac{\mu kZe^2}{\left(\frac{h}{2\pi}\right)^2} = \frac{Z}{a_0} \quad a_0 = \frac{\epsilon_0 h^2}{\pi \mu e^2} = 0,529 \text{ \AA: Bohr radius} \quad k = 1/(4\pi\epsilon_0)$$

$$\lambda^2 = -\frac{2\mu E}{\left(\frac{h}{2\pi}\right)^2} \quad E = -\frac{\left(\frac{h}{2\pi}\right)^2 \lambda^2}{2\mu}$$

$$E = -\frac{Z^2 (ke^2)^2 \mu}{2\left(\frac{h}{2\pi}\right)^2} = -Z^2 E_1 \quad E_1 = \frac{1}{2} \left(\frac{ke^2}{\frac{h}{2\pi}c}\right)^2 \mu c^2 \approx 13,6 \text{ eV}$$

$$E = -\frac{\mu Z^2 e^4}{8\epsilon_0^2 n^2 h^2} \quad (\text{as the Bohr Theory for the energy levels})$$

$$E_n = -\frac{Z^2 E_1}{n^2} \quad E_1 \approx 13,6 \text{ eV}$$

$$\lambda = \frac{Z}{na_0} \quad R = N_0 e^{-\lambda r} \quad R = N_0 e^{-Zr/na_0} \text{ where the constant } N_0 \text{ is obtained by normalization.}$$

The general solution for the radial function is as follows:

$$R_{nl} = e^{-\frac{Zr}{na_0}} \left(\frac{2Zr}{na_0}\right)^l L_{nl} \frac{2Zr}{na_0}$$

where L_{nl} is the Laguerre polynomials.

The function for the Hydrogen atom is as follows:

$$\psi_{nlm}(r, \theta, \Phi) = C_{nlm} R_{nl}(r) f_{l|m|}(\theta) e^{im\Phi} \quad \text{where } m=m_l$$

$f_{l|m|}(\theta)$ are the Legendre functions and C_{nlm} are the normalization constants.

$$E_{op} \psi_{nlm}(r, \theta, \Phi) = -\frac{Z^2 E_1}{n^2} \psi_{nlm}(r, \theta, \Phi)$$

$$L_{op}^2 \psi_{nlm}(r, \theta, \Phi) = l(l+1) \left(\frac{h}{2\pi}\right)^2 \psi_{nlm}(r, \theta, \Phi)$$

$$L_{z,op} \psi_{nlm}(r, \theta, \Phi) = m \left(\frac{h}{2\pi} \right)^2 \psi_{nlm}(r, \theta, \Phi)$$

The quantum number n , l and m are as follows:

$$n=1,2,3,\dots \quad l=0,1,2,\dots,(n-1) \quad m=-l,-l+1,\dots,0,1,2,\dots,+l$$

The energy depends only of the number n but some functions has the same value of energy. It .

The lowest energy has the value of $n=1$ $l=0$ and $m=0$. The wave function for the Hydrogen Atom is spherical with symmetry [16]. It is only function of the radius between the electron and the proton [5]. It

$$\text{is given by the next formula: } \psi_{100}(r, \theta, \Phi) = C_{100} e^{-\frac{Zr}{a_0}}$$

The constant C_{100} is obtained by normalization where φ is a probabilistic function: $\int \varphi^2 dV = 1$

$$\int \psi^* \psi dV = \iiint \psi^* \psi r^2 \sin\theta d\theta dr d\Phi = 1 \text{ in spherical coordinates}$$

The angle integration gives the value of 4π : $dV=4\pi r^2 dr$. The integration over r gives the next result:

$$C_{100} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2}$$

$$\varphi = \sqrt{\frac{Z^3}{\pi a_0^3}} e^{-Zr/a_0}$$

The probability to find the electron inside of the volume dV is $\psi^* \psi dV$. The probability to find the electron between r and $r+dr$ where $dV=4\pi r^2 dr$ is obtained as follows:

$$P(r)dr = \psi^* \psi 4\pi r^2 dr = 4\pi r^2 C_{100}^2 e^{-\frac{2Zr}{a_0}} dr$$

$P(r)$ has the maximum value in $r=a_0/Z$ which is the Bohr radius.

The expected value of r can be calculated. It is as follows:

$$\langle r \rangle = \int r \varphi^2 dV = \frac{4}{a_0^3} \int_0^\infty r^3 e^{-2r/a_0} dr = \frac{3}{2} a_0 \quad \varphi^2 = \psi^* \psi$$

The Bohr radius is obtained with the calculation of r^{-1} as follows:

$$\langle r^{-1} \rangle = \int \frac{1}{r} \varphi^2 dV = \frac{4}{a_0^3} \int_0^\infty r e^{-2r/a_0} dr = \frac{1}{a_0} \quad r=a_0$$

The probability to find the electron inside of the nucleus of radius R_0 is given by the next formula:

$$P = \int_0^{R_0} \varphi^2 dV = \frac{1}{\pi a_0^3} \int_0^{R_0} 4\pi r^2 e^{-2r/a_0} dr \cong \frac{4}{3} \frac{R_0^3}{a_0^3}$$

where R_0 is the radius of the Hydrogen nucleus: 10^{-15} m and $a_0=0,528 * 10^{-10}$ m

Thus, there is a very small probability to find the electron at the nucleus.

At the Bohr model, the electron remains in a definite orbit with $r=a_0$. At the Schrödinger model, the electron can be in any value from 0 to ∞ but the radius most probable is a_0 . The probability to find the electron in other radius is very low. The electron is considered as a charged cloud with charge: $e\psi^*\psi$ [16]. At the Bohr model the angular momentum is $\frac{h}{2\pi} (n=1) L = n \frac{h}{2\pi}$ but at the Schrödinger model the angular momentum is zero ($l=0, n=1$) $L = \sqrt{l(l+1)} \frac{h}{2\pi}$.

For the first excited state: $n=2, l=0, l=1$. For $l=0, m=0$, the function is spherical:

$$\psi_{200} = C_{200} \left(2 - \frac{Zr}{a_0}\right) e^{-\frac{Zr}{2a_0}}$$

For $l=1, m=0, m=+1, m=-1$. The functions are as follows:

$$\psi_{210} = C_{210} \left(\frac{Zr}{a_0}\right) e^{-\frac{Zr}{2a_0}} \cos\theta$$

$$\psi_{21\pm 1} = C_{211} \left(\frac{Zr}{a_0}\right) e^{-\frac{Zr}{2a_0}} \sin\theta e^{\pm i\Phi}$$

In resume, at this theory, it is no necessary to use postulates ad hoc or patches to obtain the quantization energy. It is obtained directly from the Schrödinger Equation. Also, the Schrödinger Theory doesn't use classic concepts. Besides, the magnitude of the angular momentum is quantized: $L =$

$$\sqrt{l(l+1)} \frac{h}{2\pi} \quad l=0,1,2,3,\dots,n-1$$

For l very large, the quantization of the angular momentum of the Bohr Model: $L = l \frac{h}{2\pi}$ is in accordance with the Schrödinger Theory.

The component of the angular momentum in the direction of the external magnetic field or z direction is quantized: $L_z = m_l \frac{h}{2\pi} \quad m_l=0, \pm 1, \pm 2, \dots, \pm l$

At the Normal Zeeman Effect and the Anomale Zeeman Effect, the electron has additional energy sub-levels due the interaction between the orbital magnetic dipole momentum and the magnetic dipole momentum of the spin with the external magnetic field.

They are additional interactions to the potential interaction V of the electron with the nucleus.

The magnitude of the angular momentum of the spin is also quantized:

$$L_s = \sqrt{s(s+1)} \frac{h}{2\pi} \quad s=1/2: \text{ spin orbital number}$$

$$\text{For very large } s: L_s = s \frac{h}{2\pi} \quad s=\frac{1}{2}$$

The component of the angular momentum of the spin in the direction of the external magnetic field or z direction is also quantized:

$$L_{sz} = m_s \frac{h}{2\pi} \quad m_s = \pm 1/2 \quad m_s: \text{spin number}$$

The spin is the result of applying Relativity Theory to the electron. It was done by Dirac in 1928. Then, the analogy of the electron as a sphere in rotation is not exact but it serves as model to explain the quantization of the spin. Besides, the spin has not been observed experimentally. It is only possible to say that the spin is due an intrinsic motion of the electron [4], [5].

9. An electron orbiting the nucleus

The mass of the electron is m and the mass of the nucleus is M . During the first research about the atom, the Rutherford Model was represented as the electron moves around the nucleus in a circular motion with radius R . After, the motion of the electron was represented as an ellipse as the Somerfield Model has established [4], [5], [6]. The nucleus is at the focus of the ellipse as the sun in one focus at the Planetary System [4], [5], [7], [8]. There is a strong analogy between the Planetary System and the Atom System at this model.

Fig.32. An electron orbiting the nucleus due the Electric Force

The electrical force between the electron and the nucleus gives out the Electrical Potential Energy. At the Planetary System, the gravitational force between the planets and the sun gives out the Gravitational Potential Energy. Besides, the electron only emits electromagnetic energy or photons at the jump from one stationary orbit to another stationary orbit at the atom. Then, the mass of the electron decreases due the emission of the electromagnetic energy. As result of it, the electron changes its stationary orbit by decreasing the radius R with the nucleus. Afterwards, the electron starts to move in a circular or elliptical motion (rotational motion) around the nucleus due the initial velocity of the electron but without the emission of electromagnetic energy.

9.1. Variant Mass for the electron due the Electrical Potential

$$dU = -dW \quad dW = FdR \quad F = -k \frac{e^2}{R^2}$$

The electrical potential energy is equal to the negative work done by the electrical force because it is necessary to give energy or to do work on the system to separate the electron from the nucleus.

$$c^2 dm = dU \quad c^2 dm = k \frac{e^2}{R^2} dR$$

$$c^2 \int_{m_0}^m dm = k e^2 \int_{R_i}^{R_f} \frac{dR}{R^2} \quad c^2(m-m_0) = -k e^2 \left(\frac{1}{R_f} - \frac{1}{R_i} \right)$$

$$m = m_0 - \frac{k e^2}{c^2} \left(\frac{1}{R_f} - \frac{1}{R_i} \right) \quad mc^2 = m_0 c^2 - k e^2 \left(\frac{1}{R_f} - \frac{1}{R_i} \right)$$

$$mc^2 = m_0 c^2 - \frac{k e^2}{R} \quad \text{electron mass-energy due the electrical potential}$$

$c^2 dm = dV$ and by doing the integration:

$$mc^2 - m_0 c^2 = V, \text{ then } mc^2 = m_0 c^2 + V \quad E = m_0 c^2 + V$$

which is the formula for the Electrical Potential Energy: $V = mc^2 - m_0 c^2$

$$V = mc^2 - m_0 c^2 = -k e^2 \left(\frac{1}{R_f} - \frac{1}{R_i} \right)$$

$$V = -\frac{k e^2}{R} \quad \text{classical electrical potential energy}$$

$$U = -\frac{GMm_0}{R} \quad \text{classical approach for the gravitational potential energy}$$

V increases (less negative) when R increases. If we want to separate the electron m from the nucleus M , it is necessary to apply an external force or to give an additional energy to the system. The work done by this force produces an increase of the electrical potential energy.

Part of the work done by this force or the additional energy given produces a decrease of the kinetic energy and the electron has less velocity. Nevertheless, the electron has restricted positions or radius to do the transitions from one orbit to another until it gets the stationary orbit with stationary energy level. At these stationary orbits or states, the electron doesn't emit electromagnetic energy or photons.

The electron only does the emission of the electromagnetic energy or photons at the transition from one orbit to another.

V decreases (more negative) when R decreases. If we want to reduce the distance of the electron m and the nucleus M by doing a transition from one orbit to another orbit, it is necessary that the electron m emits energy (emission as electromagnetic energy or photons) at this transition.

The emission of this energy produces a decrease of the electrical potential energy (more negative). It produces also an increase of the kinetic energy and the electron has more velocity.

9.2. Variant Mass for the Electron due to the Kinetic Energy

The change of the kinetic energy of the particle (electron) dK is transformed in an increasing of the relativistic mass-energy $dE=c^2dm$ (by using the famous formula for the energy-mass for every particle: $E=mc^2$). Therefore, it is obtained: $dE=dK \quad c^2dm = dK$

$$dK = dW = Fds = \left(\frac{dp}{dt}\right) ds = dp \left(\frac{ds}{dt}\right) = d(mv)v = v^2dm + mv dv$$

By replacing this expression in dK , it is obtained:

$$c^2dm = v^2dm + mv dv \quad c^2dm = v^2dm + mv dv$$

$$(c^2 - v^2)dm = mv dv \quad \frac{dm}{m} = \frac{v}{(c^2 - v^2)} dv$$

By doing the respective integration, it is obtained:

$$\int_{m_0}^m \frac{dm}{m} = \int_0^v -\frac{2v}{2(c^2 - v^2)} dv$$

$$\int_{m_0}^m \frac{dm}{m} = \int_{c^2}^{c^2 - v^2} -\frac{du}{2u} \quad u = c^2 - v^2 \quad du = -2v dv$$

$$\ln(m) - \ln(m_0) = (-1/2)[\ln(c^2 - v^2) - \ln(c^2)]$$

$$\ln(m/m_0) = \ln[(c^2 - v^2)/c^2]^{-1/2}$$

$$m/m_0 = [(c^2 - v^2)/c^2]^{-1/2}$$

$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}} \quad \text{relativistic electron mass due the kinetic energy}$$

At this formula, when the velocity v is increasing, the relativistic mass m is increasing. If v approximates to the light velocity $v \approx c$, then the value of mass is approaching infinity. Then, the velocity v can never get the light velocity because it implies that the mass increases to ∞ .

$$m = m_0 \left(1 + \frac{1}{2} \frac{v^2}{c^2} + \frac{3}{8} \frac{v^4}{c^4} + \dots\right) \quad m = m_0 \left(1 + \frac{1}{2} \frac{v^2}{c^2}\right) \quad v \ll c$$

$$mc^2 = m_0c^2 + \frac{1}{2}m_0v^2 \quad \text{classic approach for the mass of the electron}$$

The electrical force is equal to the centrifugal force:

$$\frac{ke^2}{R^2} = m_0 \frac{v^2}{R} \quad \frac{ke^2}{2R} = \frac{1}{2}m_0v^2$$

$$mc^2 = m_0c^2 + \frac{ke^2}{2R} \quad \text{classic approach for the mass of the electron}$$

The kinetic formula is obtained as follows:

$$c^2 dm = dK$$

and by doing the integration:

$$mc^2 - m_0c^2 = K, \text{ then } mc^2 = m_0c^2 + K \quad E = m_0c^2 + K$$

which is the formula for the kinetic energy: $K = mc^2 - m_0c^2$

$$K = m_0c^2 \left(\frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} - 1 \right) \quad K = m_0c^2 \left(\left(1 - \frac{v^2}{c^2} \right)^{-1/2} - 1 \right)$$

For higher velocities (when v is approaching to c), it is necessary an infinity kinetic energy to bring the particle to those velocities. If the particle decreases the radius orbit, the velocity and the kinetic energy increases. Nevertheless, there is a limit of the velocity for the particle which is the light velocity.

For very low velocities, it is obtained:

$$\left(1 - \frac{v^2}{c^2} \right)^{-1/2} = 1 + \frac{1}{2} \frac{v^2}{c^2} + \frac{3}{8} \frac{v^4}{c^4} + \dots \quad K = m_0c^2 \left(1 + \frac{1}{2} \frac{v^2}{c^2} + \frac{3}{8} \frac{v^4}{c^4} + \dots - 1 \right)$$

$\frac{3}{8} \frac{v^4}{c^4}$ and other terms are neglected for very low velocities $v \ll c$:

$$K = \frac{1}{2} m_0 v^2 \quad \text{kinetic energy for low velocities}$$

$$\frac{ke^2}{2R} = \frac{1}{2} m_0 v^2 \quad \& \quad K = \frac{ke^2}{2R} \quad \text{kinetic energy for low velocities}$$

9.3. Total Variant Mass for an electron which emits Electromagnetic Energy: Classical Approach

$$m_0c^2 - mc^2 = \frac{ke^2}{R} \quad \text{electrical potential energy}$$

$$m_0c^2 - mc^2 = -\frac{ke^2}{2R} \quad \text{kinetic energy}$$

Therefore, the total lost mass is given by adding the contribution of the electrical potential energy with the kinetic contribution to the mass.

$$m_0c^2 - mc^2 = \frac{ke^2}{R} - \frac{ke^2}{2R}$$

$$\Delta mc^2 = m_0c^2 - mc^2 = \frac{ke^2}{2R} \quad \text{total decrease mass of the particle}$$

$$mc^2 = m_0c^2 - \frac{ke^2}{2R} \quad \text{total mass of the particle: classical approach}$$

The total variant energy is given by the same expression of the total decrease mass of the electron in an electrical field because of the Energy Mass Law $E = mc^2$. It is due that the total variant energy correspond to the bound energy of the system (electron-nucleus) which after is emitted as electromagnetic energy or

photons and corresponds to the decrease mass of the particle. Therefore, it is obtained: $c^2 dm = dE$
 $mc^2 - m_0c^2 = E$, then $mc^2 = m_0c^2 + E$

which is the formula for the total energy E: $E = mc^2 - m_0c^2$

$$mc^2 = m_0c^2 - \frac{ke^2}{2R} \quad E = mc^2 - m_0c^2$$

$$E = \left(-\frac{ke^2}{2R} \right) \text{ total bound energy of the electron at the atom}$$

Other form to obtain the formula is as follows:

$$E = K + U$$

$$E = \frac{1}{2}mv^2 - \frac{ke^2}{R} \quad E = \frac{ke^2}{2R} - \frac{ke^2}{R}$$

$$E = -\frac{ke^2}{2R} \text{ Total Bound Energy of the electron at the atom}$$

The total bound energy is negative and equal to the kinetic energy in absolute value for the case of circular orbits. Also, the kinetic energy is positive and equal to the half of the electrical potential energy in absolute value. This total bound energy corresponds to the value of the total decrease mass of the electron when it emits electromagnetic energy or photons at the atom.

9.4. Formula development of the total mass of the electron at the electric potential of the nucleus and quantization formula

$$c^2 dm = \frac{dp}{dt} ds + \frac{ke^2}{R^2} dR \quad c^2 dm = v dp + \frac{ke^2}{R^2} dR \quad v = ds/dt$$

$p = mv$ $m = p/v$ The electrical force is equal to the centrifugal force:

$$\frac{ke^2}{R^2} = m \frac{v^2}{R} \quad \frac{ke^2}{R^2} = \frac{pv}{R}$$

$$\frac{ke^2}{R} = pv \quad -\frac{ke^2}{R^2} dR = p dv + v dp$$

$$\frac{ke^2}{R^2} dR = -p dv - v dp \quad c^2 d\left(\frac{p}{v}\right) = v dp - p dv - v dp$$

$$c^2 d\left(\frac{p}{v}\right) = -p dv \quad c^2 \frac{v dp - p dv}{v^2} = -p dv$$

$$-c^2 \frac{dp}{v} = p \left(1 - \frac{c^2}{v^2}\right) dv \quad -c^2 \frac{dp}{p} = v \left(1 - \frac{c^2}{v^2}\right) dv$$

$$\ln \frac{p}{p_0} = -\left(\left(\frac{v^2 - v_0^2}{2c^2}\right) - (\ln v - \ln v_0)\right)$$

$$\frac{p}{p_0} = \frac{v}{v_0} e^{-\left(\frac{v^2 - v_0^2}{2c^2}\right)} \quad p = mv \quad p_0 = m_0 v_0$$

$$\frac{mv}{m_0 v_0} = \frac{v}{v_0} e^{-\left(\frac{v^2 - v_0^2}{2c^2}\right)}$$

$$m = m_0 e^{-\left(\frac{v^2 - v_0^2}{2c^2}\right)} \quad \text{total relativistic mass of the electron at the atom}$$

$$\Delta m = m_0 c^2 - mc^2 = m_0 c^2 \left(1 - e^{-\left(\frac{v^2 - v_0^2}{2c^2}\right)}\right) \quad \text{total decrease mass of the electron at the atom}$$

If $v^2 \ll c^2$, then it is obtained for the classical case:

$$e^{-\left(\frac{v^2 - v_0^2}{2c^2}\right)} = 1 - \left(\frac{v^2 - v_0^2}{2c^2}\right) + \frac{\left(\frac{v^2 - v_0^2}{2c^2}\right)^2}{2!} + \dots$$

$$\frac{\left(\frac{v^2 - v_0^2}{2c^2}\right)^2}{2!} \text{ and other terms are neglected}$$

$$\frac{ke^2}{R^2} = m \frac{v^2}{R} \quad \frac{ke^2}{mR} = v^2 \quad m = m_0 \left(1 - \left(\frac{v^2 - v_0^2}{2c^2}\right)\right)$$

$$\left(\frac{v^2 - v_0^2}{2c^2}\right) = \frac{ke^2}{2m_0 c^2} \left(\frac{1}{R} - \frac{1}{R_0}\right) \quad R_f = R \quad R_i = R_0$$

$$m = m_0 \left(1 - \frac{ke^2}{2m_0 c^2} \left(\frac{1}{R} - \frac{1}{R_0}\right)\right) \quad \text{mass of the electron: classical approach}$$

$$m_0 c^2 - mc^2 = \frac{ke^2}{2} \left(\frac{1}{R} - \frac{1}{R_0}\right) \quad \text{total decrease mass: classical approach}$$

$$m_0 c^2 - mc^2 = \frac{ke^2}{2R} \quad \text{total decrease mass of the electron: classical approach}$$

It is in accordance with the total energy for the electron (bound energy) at the atom for the classical approach which is equal to the decrease mass of the electron and equal to the electromagnetic radiation emitted by the electron at the atom. The electron at the atom only can take restricted positions which are explained by quantum mechanics.

For the total energy of the electron or bound energy, it is obtained:

$$E = mc^2 - m_0 c^2 \quad m = m_0 e^{-\left(\frac{v^2 - v_0^2}{2c^2}\right)}$$

$$E = m_0 c^2 \left(e^{-\left(\frac{v^2 - v_0^2}{2c^2}\right)} - 1\right) \quad \text{total relativistic energy for the electron in the atom}$$

If $v^2 \ll c^2$, then it is obtained for the classic case:

$$e^{-\left(\frac{v^2 - v_0^2}{2c^2}\right)} = 1 - \left(\frac{v^2 - v_0^2}{2c^2}\right) + \frac{\left(\frac{v^2 - v_0^2}{2c^2}\right)^2}{2!} + \dots$$

$$\frac{\left(\frac{v^2 - v_0^2}{2c^2}\right)^2}{2!} \text{ and other terms are neglected}$$

$$E = -m_0 \left(\frac{v^2 - v_0^2}{2}\right) \quad \text{classical approach}$$

$$\frac{ke^2}{R^2} = m \frac{v^2}{R} \quad \frac{ke^2}{mR} = v^2 \quad \left(\frac{v^2 - v_0^2}{2}\right) = \frac{ke^2}{2m_0} \left(\frac{1}{R} - \frac{1}{R_0}\right)$$

$$E = -m_0 \left(\frac{ke^2}{2m_0} \left(\frac{1}{R} - \frac{1}{R_0}\right)\right) \quad E = -\left(\frac{ke^2}{2} \left(\frac{1}{R} - \frac{1}{R_0}\right)\right)$$

$$E = -\left(\frac{ke^2}{2R}\right) \text{ total energy for the electron at the atom or bound energy}$$

The kinetic energy for the electron at the atom for the classical approach is the same formula but in absolute value: $K = \left(\frac{ke^2}{2R}\right)$

The total lost mass energy of the electron at the atom is given by the formula demonstrated and it is equal in absolute value to the total bound energy of the system which is emitted as electromagnetic energy when the electron does the transition from one orbit to another orbit with fewer radiuses. The emission of the total electromagnetic energy E produces a decrease mass of the particle: $\Delta m = E/c^2$.

If $R_f < R_i$ $\Delta E = E_f - E_i = \left(-\frac{ke^2}{2R_f}\right) - \left(-\frac{ke^2}{2R_i}\right)$ is negative, it is given out energy which means that the electron losses mass, the electron increases the kinetic energy and the velocity but decreases the electrical potential energy (more negative). Part of the lost energy (electromagnetic energy emission or photon) is given out by decreasing the potential energy and part by increasing the kinetic energy.

If $R_f > R_i$ ΔE is positive, which means that additional energy is given to the electron or additional work is done on the system, the electron decreases the kinetic energy and the velocity but increases the potential energy (less negative). Part of the work or additional energy is used to increase the potential energy and part to diminish the kinetic energy.

Therefore, the total energy for the electron at the atom for the classical approach is: $E = -\left(\frac{ke^2}{2R}\right)$

Then, it is possible to obtain all the quantization formula as it was done before:

If the radiation is emitted in the transition from the initial state i to the final state f (for example from $n=2$ to $n=1$), the difference energy of those levels is as follows: $\Delta E = E_i - E_f$ $E_i > E_f$ (E_i is less negative than E_f)

$$\Delta E = -\left(\frac{ke^2}{2} \left(\frac{1}{R_i} - \frac{1}{R_f}\right)\right) \quad \Delta E = \left(\frac{ke^2}{2} \left(\frac{1}{R} - \frac{1}{R_0}\right)\right) \quad R_i = R_0 \quad R_f = R$$

The formula of Balmer Series is as follows:

$$\frac{1}{\lambda} = R \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad n > n' \quad R = 1.099731 \times 10^7 \text{ m}^{-1}: R = \frac{me^4}{8\epsilon_0^2 ch^3} \text{ Rydberg Constant}$$

$$\frac{f}{c} = R \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad f = cR \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad f = \frac{me^4}{8\epsilon_0^2 h^3} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad \lambda = c/f$$

This formula was obtained from the quantization of the radius by using De Broglie wave-particle duality ($\lambda = h/mv$) and the adjustment of the wave of the electron at the orbit of the atom ($2\pi r = \lambda$) and the formula $\Delta E = hf$ for the energy emission of the electron at the atom.

Because $\Delta E = hf$, it is possible to obtain the formula of energy:

$$\Delta E = hf = \frac{mhe^4}{8\epsilon_0^2 h^3} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad \Delta E = \frac{me^4}{8\epsilon_0^2 h^2} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right)$$

This formula can be compared with the mass formula development for the classic approach:

$$\Delta E = \left(\frac{ke^2}{2} \left(\frac{1}{R} - \frac{1}{R_0} \right) \right)$$

$$\frac{me^4}{8\epsilon_0^2 h^2} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) = \left(\frac{ke^2}{2} \left(\frac{1}{R} - \frac{1}{R_0} \right) \right)$$

n : main quantum number of the initial state with radius R_0

n' : main quantum number of the final state with radius R

$$\frac{e^2}{4\pi\epsilon_0(2)(\frac{\epsilon_0 h^2}{\pi me^2})} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) = \left(\frac{ke^2}{2} \left(\frac{1}{R} - \frac{1}{R_0} \right) \right) \quad k = 1/(4\pi\epsilon_0)$$

$$\frac{ke^2}{2} \left(\frac{1}{(\frac{\epsilon_0 h^2}{\pi me^2})n'^2} - \frac{1}{(\frac{\epsilon_0 h^2}{\pi me^2})n^2} \right) = \left(\frac{ke^2}{2} \left(\frac{1}{R} - \frac{1}{R_0} \right) \right)$$

It is concluded that the radius must be proportional to the number n^2 .

$$R = a_0 n'^2 \quad R_0 = a_0 n^2$$

$$R = a_0 n^2 \quad a_0 = \frac{\epsilon_0 h^2}{\pi me^2} \quad a_0 = 0,529 \times 10^{-10} \text{ m} = 0,529 \text{ \AA} \quad \text{Bohr radius}$$

Besides, It is known that the radius is proportional to the main quantum number and the Bohr radius from the quantization of the radius by using the De Broglie wave-particle duality and the adjustment of the wave of the electron at the orbit of the atom: $R = \frac{\epsilon_0 h^2}{\pi me^2} n^2$.

The Constant of Rydberg is obtained as follows:

$$f = cR \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad \Delta E = hf = chR \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \quad \Delta E = \left(\frac{ke^2}{2a_0} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \right)$$

$$\text{chR} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) = \left(\frac{ke^2}{2a_0} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \right) \quad \text{chR} = \frac{ke^2}{2a_0}$$

$$R = \frac{ke^2}{2cha_0} \quad h: \text{Planck Constant} \quad a_0 = \frac{\epsilon_0 h^2}{\pi m e^2} \quad k = 1/(4\pi\epsilon_0) \quad c: \text{light velocity}$$

$$R = \frac{me^4}{8\epsilon_0^2 ch^3} \quad R = 1.0997313414 \cdot 10^7 \text{ m}^{-1} \quad \text{Rydberg Constant}$$

Besides, if we suppose that the Rydberg Constant is known from the experimental result of Balmer, then the Planck Constant is possible to obtain:

$$\text{chR} = \frac{ke^2}{2a_0} \quad h = \frac{ke^2}{2a_0 c R} \quad a_0 = \frac{\epsilon_0 h^2}{\pi m e^2}$$

$$k = 1/(4\pi\epsilon_0) = 9 \cdot 10^9 \text{ N m}^2/\text{C}^2 \quad \epsilon_0: \text{vacuum permittivity} = 8,85 \cdot 10^{-12} \text{ Farad/m}$$

$$a_0: \text{Bohr radius} = 5,3 \cdot 10^{-11} \text{ m} \quad c: \text{light velocity} = 3 \cdot 10^8 \text{ m/s}$$

$$e: \text{electron charge} = 1,6 \cdot 10^{-19} \text{ Coulomb (C)}$$

$$R = 1.097313414 \cdot 10^7 \text{ m}^{-1}: \text{Rydberg Constant}$$

By using those values, it is possible to obtain the Planck Constant:

$$h = 6,63 \cdot 10^{-34} \text{ J-s} \quad \text{Planck Constant}$$

10. Ionization emission energy of the electrons at the Hydrogen Atom and the bound of Diatomic Molecules

In order to test the mass development formula for the ionization emission energy of the electron for the Hydrogen atom, some calculation by using Quantum Mechanics are done.

After, the mass results for both methods are compared. The formulas for velocity, radius and energy for an electron at the quantized atom[6] are as follows:

$$v = \frac{Ze^2}{2\epsilon_0 nh} \quad r = \frac{n^2 h^2 \epsilon_0}{\pi m_0 Z e^2} \quad E = \frac{-Z^2 e^4 m_0}{8 \epsilon_0^2 h^2 n^2}$$

Z: atomic number of the atom e : charge of the electron

ϵ_0 : vacuum permittivity h : Planck constant

n : main quantum number, electron energy level, orbit of the electron

m_0 : rest mass of the electron

The physical constants are given in the next table:

h	$6,63 \cdot 10^{-34} \text{ J-s}$
ϵ_0	$8,85 \cdot 10^{-12} \text{ Farad/m}$
π	3,1416
m_0	$9,11 \cdot 10^{-31} \text{ kg}$
e	$1,6 \cdot 10^{-19} \text{ C}$
r_0	0,528 $\text{\AA}$

Table 3: Physical constants

First energy level Hydrogen atom: -13,6 eV $n=1$

Second energy level Hydrogen atom: -3,4 eV $n=2$

Therefore, if the electron jumps from the first level to the second level, it must gain an energy of 10,2 eV (energy difference of the two levels).

If the electron jumps from the second level to the first level, it must lose an energy of 10,2 eV. If the electron jumps from the second level to the first level, the mass of the electron must lose this equivalent mass-energy. And the lost mass of the electron (which is equivalent to the mass-energy of the electromagnetic radiation emitted) occurs during the transition from the second level to the first level converted as kinetic energy. In mathematical formulation, it is as follows: $(m_0 - m)c^2 = hf = K$

$E = hf$: energy of the photon emitted (electromagnetic radiation). It is in coincidence with the development formula for the energy emission of the electron at the atom. Thus, we are going to proceed to test the mass formula: if the electron at the first level ($n=1$) leaves from the atom, then the ionizing energy is equal to -13,6 eV. It corresponds to the energy emission of the electron. Therefore, the mass of the electron after losing this mass-energy emission is: $mc^2 = m_0c^2 - hf$

$$mc^2 = 511875 - 13,6 = 511861,4 \text{ eV}$$

For other hand, the mass electron calculation with the mass development formula is as follows:

$$m = m_0 e^{-\left(\frac{v^2}{2c^2}\right)}$$

The velocity is given by this formula:

$$v = \frac{Ze^2}{2\epsilon_0 nh}$$

It is interesting to mention that this formula doesn't include the mass of the particle. So, the orbits have specific values for the particle independent of the mass of it. By replacing the values for Z ($Z=1$), e , ϵ_0 , n ($n=1$), h , it is obtained:

$v=2181489,72$ m/s. By replacing this value at the mass formula, it is achieved:

$$mc^2=511861,4 \text{ eV}$$

It is the same value that the last calculation by using quantum mechanics. It is possible to do the same for the second level of the Hydrogen atom. The ionizing energy for electron at the second level is: $-3,4$ eV.

If the electron at the second level ($n=2$) leaves from the atom, the ionizing energy is equal to $-3,4$ eV. It corresponds to the energy emission of the electron. Therefore, the mass of the electron after losing this mass-energy emission is: $mc^2=m_0c^2-hf$

$$mc^2=511875-3,4$$

$$=511871,6 \text{ eV}$$

For other hand, the mass electron calculation with the mass development formula is as follows:

$$m = m_0 e^{-\left(\frac{v^2}{2c^2}\right)}$$

The velocity is given by this formula:

$$v = \frac{Ze^2}{2\epsilon_0 nh}$$

By replacing the values for Z ($Z=1$), e , ϵ_0 , n ($n=2$), h , it is obtained:

$$v=1090744,859 \text{ m/s}$$

By replacing this value at the mass formula, it is achieved:

$$mc^2=511871,6 \text{ eV}$$

n	v	r	$E=hf$ Ecínetica (ionization energy)	$mc^2=m_0c^2-hf$	$m = m_0 e^{-\left(\frac{v^2}{2c^2}\right)}$
1	2181489,72	5,3096E-11	-13,54798602	511861,452	511861,4671
2	1090744,86	2,1238E-10	-3,386996504	511871,613	511871,6167
3	727163,24	4,7786E-10	-1,50533178	511873,4947	511873,4963
4	545372,43	8,4954E-10	-0,846749126	511874,1533	511874,1542
5	436297,944	1,3274E-09	-0,541919441	511874,4581	511874,4587
6	363581,62	1,9115E-09	-0,376332945	511874,6237	511874,6241
7	311641,388	2,6017E-09	-0,276489511	511874,7235	511874,7238

Table 4: Values of the velocities, radius, energy of the ionization for the different levels of energy of the hydrogen atom. Also, it is showed the mass of the electron after the emission of the electromagnetic radiation by using quantum mechanics and for the development formula of the variant mass

It is the same value that the last calculation by using quantum mechanics. It is showed at the next table the values of the velocities, radius, energy of the ionization for the different levels of energy of the hydrogen atom. Also, it is showed the mass of the electron after the emission of the electromagnetic radiation by using quantum mechanics ($mc^2 = m_0c^2 - hf$) and for the formula of the variant mass for the electron at the atom after the energy emission: $m = m_0 e^{-\left(\frac{v^2}{2c^2}\right)}$. It is possible to confirm the accuracy of the formula demonstrated theoretically. Besides, the table showed that when the velocity decreases (at the different levels of energy of the Hydrogen atom) the mass increases. Also, levels which are closest to the nucleus have higher velocities than the farthest.

Bound of Diatomic Molecules

It is possible to do the analysis for the center of mass (CM) as follows:

Fig.33. Center of mass for diatomic molecules

$$mr = MR \quad R = (m/M)r \quad r' = r + R \quad r' = r + (m/M)r$$

$$r' = \frac{M+m}{M} r \quad r = \frac{M}{M+m} r'$$

$$m \frac{v^2}{r} = \frac{kZe^2}{r'^2}$$

$$v^2 = r \frac{kZe^2}{mr'^2} = \frac{M}{M+m} r' \frac{kZe^2}{mr'^2} = \frac{kZe^2}{2m_0 r'} \quad M = m = m_0$$

$$v = \sqrt{k \frac{Ze^2}{2m_0 r'}}$$

Firstly, we consider the Hydrogen molecule H_2 . The two electrons can be shared if the spins are in opposite direction. The molecule of H_2 is more stable than the molecule of ionized hydrogen H_2^+ .

The mass of H_2 is: $m_0 = 1,67353 \cdot 10^{-27}$ kg.

The nuclear separation is: $r = 0.74 \text{ \AA}$ ($1 \text{ \AA} = 10^{-10} \text{ m}$).

$$v = \sqrt{k \frac{Ze^2}{2m_0 r}} \quad k = \frac{1}{4\pi\epsilon_0} = 9 \cdot 10^9 \text{ Nm}^2/\text{C}^2 \quad Z=1 \quad e = 1,6 \cdot 10^{-19} \text{ C}$$

$$v=30499,52739 \text{ m/s}$$

$$m = m_0 e^{-\left(\frac{v^2}{2c^2}\right)} \text{ where } c \text{ is the light velocity } c=3*10^8 \text{ m/s.}$$

$$\Delta mc^2=(m_0 e^{-\left(\frac{v^2}{2c^2}\right)})c^2 - m_0 c^2$$

$$\Delta mc^2=4,8648 \text{ eV}$$

The experimental value for the bond energy for the Hydrogen molecule H_2 is 4,72 eV.

For the ionized hydrogen H_2^+ , it is obtained:

The mass of H_2^+ is approximately: $m_0=1,67353 * 10^{-27} \text{ kg}$.

The nuclear separation is: $r=1.06 \text{ A}$ ($1 \text{ A}=10^{-10} \text{ m}$).

The bound energy for the H_2^+ is less intense than for H_2 . Therefore, the nuclear separation is higher for H_2^+ than for H_2 .

$$v = \sqrt{k \frac{Ze^2}{2m_0 r}} \quad k = \frac{1}{4\pi\epsilon_0} = 9*10^9 \text{ Nm}^2/\text{C}^2 \quad Z=1 \quad e=1,6*10^{-19} \text{ C}$$

$$v=23851,53228 \text{ m/s}$$

$$m = m_0 e^{-\left(\frac{v^2}{2c^2}\right)} \text{ where } c \text{ is the light velocity } c=3*10^8 \text{ m/s}$$

$$\Delta mc^2=(m_0 e^{-\left(\frac{v^2}{2c^2}\right)})c^2 - m_0 c^2$$

$$\Delta mc^2=2,9752064 \text{ eV}$$

The experimental value for the bond energy for the Ionized Hydrogen molecule H_2^+ is 2,65 eV. The bound energy for H_2 is not the double of the bound energy for H_2^+ , because the repulsion between the electrons of the H_2 decrease the bound from 5.3 eV to 4.72 eV and the distance is 0,74 A instead of 0.53 A which is the nuclear separation of H_2^+ divided by 2: $1.06 \text{ A} / 2$.

For the O_2 , it is obtained:

The mass of O_2 is: $m_0=2,77 * 10^{-26} \text{ kg}$.

The nuclear separation is: $r=1.21 \text{ A}$ ($1 \text{ A}=10^{-10} \text{ m}$).

$$v = \sqrt{k \frac{Ze^2}{2m_0 r}} \quad k = \frac{1}{4\pi\epsilon_0} = 9*10^9 \text{ Nm}^2/\text{C}^2 \quad Z=1 \quad e=1,6*10^{-19} \text{ C}$$

$$v=5862,6459,81 \text{ m/s}$$

$$m = m_0 e^{-\left(\frac{v^2}{2c^2}\right)} \text{ where } c \text{ is the light velocity } c=3*10^8 \text{ m/s}$$

$$\Delta mc^2 = (m_0 e^{-\left(\frac{v^2}{2c^2}\right)})c^2 - m_0 c^2$$

$$\Delta mc^2 = 2,9752083 \text{ eV}$$

It is possible to calculate the rotation frequency w for the O_2 :

$$L = Iw \approx \frac{h}{2\pi}$$

$$w \approx \frac{h}{2\pi I}$$

$$I = 2m_0(r/2)^2 = 2,0277*10^{-46} \text{ kg m}^2$$

By replacing the value of the Planck constant h , it is obtained:

$$w = 5,20*10^{11} \text{ Rad/s}$$

It is in accordance with the experimental measured for the rotation frequency. The rotation frequency is lower than the vibration frequency which is in the order of 10^{13} Hz.

11. Conclusions

At this research, firstly it is demonstrated the research about the blackbody radiation of Planck, the corpuscular behavior of the radiation (Photoelectric and Compton Effect, Pair Production, Fluorescence, Moseley Plot), the spectral lines of Balmer, the research at the atom of Brown, Rutherford, Bohr, Schrödinger, Heisenberg with the all development of the quantum mechanics, the quantum numbers and atoms with more than one electron. Besides, it is explained why the electron doesn't radiate energy as a particle and a wave and why the electron has restricted radius for the motion at the atom. Also, it is demonstrated the wave-particle duality of De Broglie and the Heisenberg Uncertainty Principle, Diffraction by using a Fourier Approach and Interference Double Slit Experiment by using the wave behavior of the electron. It is also demonstrated the energy levels for the Hydrogen atom by using the Schrödinger Equation.

Planck's great contribution (1901) consisted in proposing that the experimental results of the blackbody radiation could be obtained if the average energy was treated as a discrete variable instead of the continuous variable of classical physics [9]. The quantization of the energy of the electron oscillators of the blackbody cavity was a great advance for the atom research.

Then Rutherford proposed a planetary system for the explanation of the experiment of Geiger and Marsden. This experiment only can be explained if the nucleus is constituted by a nucleus of positive

charge with the electrons with negative charge moving around it at a large distance or radius respect to the nucleus [4], [5], [8]. But, the electrons will radiate electromagnetic energy in a continue form. As consequence of it, the electrical force will put the electrons towards the core of the nucleus [4]. Besides, it will result in a continuous spectrum of energy emission of the electron and in an instability of the atom (atom collapse) and the matter in general. But, it doesn't occur in the reality: there is a discrete spectrum of energy emission of the electron at the atom and there is stability at the atom. Then, it was necessary to obtain other model to explain this fact.

Bohr proposed a model with some postulates to solve the instability of the atom. At this article, it is explained the postulates of Bohr and the reasons for them by using De Broglie approach. Also, it is explained by using the development formula for the variant mass of the electron at the atom. Bohr postulated the quantization of the energy transition for the electrons at the atom and the quantization of the angular momentum. Bohr could explain the atom stability (the no radiation for the electrons at the atom) with those postulates and obtain a formula for the quantization of the energy, velocity, radius, angular momentum, frequency and wavelength of the radiation emitted or absorbed.

Later, the modern quantum physics could explain the postulates of Bohr and obtain the quantization formula for the energy and angular momentum at the stationary levels by applying the Schrödinger Theory (wave probabilistic theory) and Heisenberg Theory (matrix theory) [4], [5]. The duality wave-particle of De Broglie and the Heisenberg Uncertainty Principle were support for the development fo the modern quantum physics. The stationary states or levels correspond to those functions which satisfy the Schrödinger Equation [4], [5]. The electron in an atom no excited is at rest. Thus, it cannot radiate energy because it corresponds to a stationary level of the atom [4], [5].

At this research, it is to demonstrated the discovery formula which describe exactly the variant mass of a charged particle as the electron at the atom which emits electromagnetic energy from one stationary level to other. The formula is in agreement at the classic limit for the bound energy for the particle orbiting the nucleus at the classic limit. The results of the formula are compared with the ionization energy emission for the electron at the atom and the bound energy for the diatomic molecules. The results of the theoretical formula are in agreement with the experimental results with high accuracy.

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