

X Rays and Electron Diffraction & Interference and Diffraction for the electron by using the Fourier Approach and Wave Properties, The Variant Mass of the Electron at the atom & The Variant Mass for an Accelerated Charged Particle (Maxwell Radiation)

#### Giovanni Alcocer

Independent Research, Guayaquil, Ecuador. Email: giov\_alc\_science@hotmail.com



Master in Physics with Specialization in Astrophysics and Medical Physics, Professor of Physics, Advanced Mathematics and Science in general, Author of the recognized and renowned articles: The Fundaments of the Mass: Gravitation, Electromagnetism and Atom.

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#### ABSTRACT

The X rays Diffraction Experiment covers: theory, interaction of photons with the matter, sources of x rays, x rays tube, radioactivity, x rays detector, x rays diffraction process, crystals, miller indices and Bravais lattices, Bragg reflection on crystal, symmetry elements, point group of symmetry, fourteen bravais lattices, crystalline systems bravais, 32 crystalline punctual groups, stereogram of the 32 crystalline punctual groups, brillouin zone and the cubic system lattice, real space (direct lattices) and the reciprocal space (reciprocal lattices), the Laue experiment of x rays diffraction on crystal, experimental set up, scintillators and photomultipliers. Besides, it is researched the Electron Diffraction and the Diffraction and Interference for the electron by using the Fourier Approach and Wave Properties, Diffraction: Heisenberg's Uncertainty Principle, Uncertainty Principle of Heisenberg by applying wave properties, Interference: Double Slit Experiment, The Copenhagen Interpretation, Pilot wave interpretation and why the electron doesn't radiate energy as a particle.

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 seimen Energienhalt abhängig?): "If a body emits energy E in the form of radiation, its mass decreases by  $E/c^2$ ". The fact that the energy that leaves from the body is converted into radiation energy makes no difference, so the more general conclusion is reached that the mass of a body is a measure of the content of its energy... It is not impossible that with bodies whose content of energy is highly variable (for example radio salts) the theory can be successfully tested. If the theory corresponds to the fact, radiation conducts inertia between the bodies that emit and absorb it<sup>1</sup>".

This is true for any type of radiation emitted (gravitational or electromagnetic energy) which produces a decrease in the mass of the body. Respect to the gravitational energy emission, it is demonstrated by theory, experiment and result the discovery formula which describe exactly the variant mass of a particle which emits gravitational energy which was demonstrated by myself at the article: The Fundament of the Mass and Effects of the Gravitation on a Particle and Light in the mass, time, distance, velocity, frequency, wavelength: Variant Mass for a Particle which emits Gravitational Energy for a particle orbiting a large Planet or Sun and for a Binary Star and Variant Frequency for the Light passing close a Gravitational Field from a Massive Object (Sun).

The results of the mass formula are of great relevance for Gravitational Interactions. It is in accordance with the classic result for the emission of the total gravitational energy (bond total energy) for a particle orbiting a large Planet or Sun and for a Binary Star. 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 demonstrated the development formula for the variant mass of the electron at the atom which describe exactly the variant mass of the electron (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. Besides, Maxwell's theory shows that electromagnetic waves are radiated whenever charges accelerate as for example for the electrón. 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.

Therefore, an additional objective of this article is to demonstrate by theory, calculations and results the discovered formula which describe exactly the variant mass of an accelerated charged particle. This charged particle emits electromagnetic radiation which is called the Maxwell Radiation. Also, the article analyzes and establishes about the effects of the variant mass on the particle. In addition, the formula is tested with the electromagnetic radiation emitted for an electron when leaves from the atom. Finally, it is obtained the formula for the power energy emitted for an Accelerated Charged Particle.

**Keywords:** Interaction of photons with the matter, X rays, radioactivity, X ray detector, X rays diffraction process, Crystals, Miller indices, Bravais lattices, Bragg reflection on crystal, Symmetry elements, Point group of symmetry, Fourteen bravais lattices, Crystalline systems bravais, 32 crystalline punctual groups, Stereogram of the 32 crystalline punctual groups, Brillouin zone and the cubic system lattice, real space (direct lattices) and the reciprocal space (reciprocal lattices), the Laue experiment, scintillators and photomultipliers, Variant mass, Ionizing energy atom, Maxwell theory, Einstein mass-energy, Accelerated charged particle, Electromagnetic radiation, Ionizing energy atom, Power energy.



## 1. Introduction

### 1.1. Interaction of photons with the matter

The interaction of photons with the matter is characterized by the fact of that each x ray photon is removed individually from the incident beam in a single event [1]. [2]. Thus, the number of photons removed  $\Delta B$ , is proportional to the traversed thickness  $\Delta x$ , and to the number of incident photons B:

 $\Delta B = -\mu B\Delta x$  ( $\mu$ : proportionality constant called the attenuation coefficient).

The absorption occurs if only a certain fraction of the radiation ( $B_o$ ) passes through the absorber. If it happens, the wavelength of the transmitted beam is unchanged and the transmitted beam B (if the radiation is homogeneous,  $\mu$  is a constant) is described by the next formula (which is called attenuation of the radiation in matter) [45]:

 $B = B_0 e^{-\mu x}$ 

A number of photons equal to  $(B_0-B) = B_0(1-e^{-\mu x})$  have been lost in the absorption process, most of this loss being due to the photoelectric effect. The value of the  $\mu$  constant referred in the above equation is a function of both: the photoelectric absorption ( $\tau$ ) and the scatter radiation ( $\sigma$ ):  $\mu = f(\tau) + f(\sigma)$ 

However,  $f(\tau)$  is usually large in comparison with  $f(\sigma)$ .

Because the photoelectric absorption is made up of the absorption in the various atomic levels, it is a dependent function of the atomic number. A plot of  $\mu/\rho$  against  $\lambda$  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 [1]-[4], [45].



Fig.1. Mass attenuation coefficient  $(\mu/\rho)$  as a function of the energy for several elements [45]

In the energy range from about 50 keV to about 50 MeV, the most of the interactions are due to:

### (a) Coherent (Rayleigh) effect

This effect occurs only with a low energy of the incident photon. We have only scattering of the incident photon and no ionization. The x-ray photon collides with one of the electrons of the absorbing element and no energy is



lost in the collision process (so, the scattered radiation will retain exactly the same wavelength as the incident beam) [1], [2], [3], [4], [45]. The probability of this effect is proportional to  $\frac{Z^{2.6}}{E^2}$ .

## (b) Photoelectric Effect (Quantization of the radiation: light)

For the energy range in the X-Rays experiment the photoelectric effect is dominant. It occurs for low energy photons E<200 keV. This effect can be explained at the microscopic level by means of the electromagnetic radiations as composed of photons. Thus, an incident photon with sufficient energy is completely absorbed by an bound electron of the atom in the absorber material, and the electron is ejected (photoelectron). Thus, the photon gives all its energy to a bound electron (recoil electron) of the atom (bound electron is required in order to conserve the energy and the momentum), which 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 orbit or by a free electron from outside of the atom [1], [2], [3], [4].

Then, the transition of the electron from a higher shell is accompanied by an emission of a x-ray or this x-ray emitted can be imparted to another electron, which is emitted and it is called Auger electron. The subject of this study is called Fluorescence. The interaction is again dependent of Z, and an approximate expression for the absorption probability  $\tau$  is proportional to  $\frac{Z^n}{E^{3.5}}$  where, n is normally between 4 and 5 depending of the absorbing material.

The Photoelectric Effect can also be explained by the wave theory in 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 therefore, they can be emitted [1], [2], [3], [4], [45].

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:  $hf=K_{max}+U_o$  where  $U_o$  is the bound energy of the electron, hf is the electron energy and  $K_{max}$  is the maximum kinetic energy of the electron [1], [2], [3], [4], [45].

The bound energy  $U_o$  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:  $hf_{min}=U_o$   $f_{min}=U_o/h$   $U_o=$  work function K=0 for  $f_{min}$ .

If  $f < U_o/h$  (very low frequency, very low energy), then there is no electron ejected independent of the radiation intensity. If the frequency is increased until the value where the energy of a single photon E=hf is more than the bound energy of the electron or work function  $U_o$ :  $hf \ge U_o/h$ , 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  $f>U_o/h$ ) increases, then more electrons can be ejected.



The maximum kinetic energy of the electron increases linearly with the frequency:  $K_{max}$ =hf-U<sub>o</sub>. Then, it 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 quantitated as discrete quantum energy called photons [1], [2], [3], [4], [45].

In resume, this Photoelectric 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 emitted.

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], [45]. It was also possible to determine Planck's constant with this experiment [5], [45].



Fig.2. Graphic of the maximum kinetic energy of the photoelectrons versus the frequency of the light for the Photoelectric Effect

The Fig shows a linear relationship between the maximum kinetic energy and the frequency:  $K_{max}$ =hf-U<sub>o</sub>. 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:

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

V<sub>max</sub>: electrical potential necessary to stop the electron flux: retardation potential.

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



s=h/e (s: slope)

h=se 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], [45].

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

## (c) Compton Scattering (Incoherent Scattering)

At energies much greater than the binding energies of the electrons, the photons are scattered as if the electrons were free and at rest. In this case, an incident photon scatters from an outer shell electron in the absorber material at an angle  $\Phi$ , and part of the photon energy is imparted to the electron as kinetic energy. Typically, the photon will have sufficient energy to produce several recoil electrons. Then, in a x-ray beam all possible energy losses will occur. The net result is the production of ion cascades as fast electrons react with other atoms. 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. It is the dominant mode of interaction around 1 MeV (intermediate energy range) [1], [2], [3], [4], [45].

The probability decreases rapidly with the increasing energy and it is also dependent on the number of electrons available for the scattering of the photon, and hence it increases proportionally with the increasing atomic number Z. Thus, the probability of this effect is proportional to Z/E. 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. It extends up to an energy corresponding to the maximum energy transfer, where there is a sharp cut-off point, known as the Compton Edge [1], [2], [3], [4], [45].

#### (d) Pair Production

Pair production (high energy  $\gamma$  rays (photons) from 5 to 10 MeV) is the process in which a photon in the field of a nucleus or an electron disappears with the creation of an electron-positron pair.



Fig.3. Relative probability (set by  $\sigma$ : cross section) of each type of interactions as a function of energy in lead [45]



The total kinetic energy of the resultant particles is equal to the photon energy minus the mass energy of the two particles which have been created. The cross section for this process shows that it varies with Z approximately as  $Z^2$  and increases with increasing photon energy. For materials with higher atomic number Z, this dominance will occur at lower energies. If the energy of the incident photon is greater than 1.022 MeV (twice the electron rest mass) in the presence of an atomic nucleus, then an electron/positron pair can be produced. Any residual energy is distributed evenly between the electron and the positron as kinetic energy. Afterwards, the positron is annihilated with one of the atomic electrons producing two  $\gamma$  rays of energy 511 keV [1], [2], [3], [4], [45].

## 1.2. X-Rays Theory and X-Rays Fluorescence process

The X-rays can be described in 2 forms: electromagnetic wave or particle (photon). The photon energies of the X-rays (in the electromagnetic spectrum) are between 100 eV and 100 keV, the wavelengths between  $10^{-8}$  m and  $10^{-12}$  m, and the frequencies between  $10^{16}$  Hz and  $10^{20}$  Hz.

The X-rays were discovered by Wilhelm K. Roentgen in 1895 and in 1913 Henry Moseley measured and plotted the x-rays frequencies for about 40 of the elements of the periodic table. Moseley showed that the  $K_{\alpha}$  X-rays followed a straight line when the atomic number Z versus the square root of the frequency v was plotted [5], [8], [9], [45]. We can write his empirical relationship as follows:

$$hv_{K\alpha} = 13.6 \text{ eV} (Z - 1)^2 \left(\frac{1}{1^2} - \frac{1}{2^2}\right) = \frac{3}{4} 13.6 (Z - 1)^2 \text{eV}$$

$$Z = \sqrt{\frac{4hv_{K\alpha}}{3(13.6)*1.6*10^{-19}}} + 1$$
 (atomic number versus frequency v in Hz)

$$Z = \sqrt{\frac{v_{K\alpha}}{0.246 * 10^{16}}} + 1 = 2.02\sqrt{\frac{v_{K\alpha}}{10^{16}}} + 1$$
$$Z = 2,016 * 10^{-8}\sqrt{v_{K\alpha}} + 1$$

With the insights from the Bohr model, we can write this empirical relationship as follows:

 $\Delta E = hcR(Z - 1)^2 \left(\frac{1}{n^2} - \frac{1}{n^2}\right) \qquad R = \frac{me^4}{8\varepsilon_0^2 ch^3} : \text{Rydberg Constant}$ 

 $\Delta E = hv = hcRZ^2(\frac{1}{n'^2} - \frac{1}{n^2})$  energy spectral lines

hcR: Rydberg in unit of energy=13.6 eV

(Z- $\sigma$ )=(Z-1)  $\sigma$ =1: shielding constant ( $\sigma$ ≤1) n'=1 n=2: K $\alpha$  lines

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

$$Z = \sqrt{\frac{4h}{(3)(13,6)}} \sqrt{v_{K\alpha}} + 1$$
$$Z = 2,016 * 10^{-8} \sqrt{v_{K\alpha}} + 1$$

Z versus  $\sqrt{v_{K\alpha}}$ : Moseley Plot



Fig.4. Moseley's plot: atomic number Z vs square root of frequency

 $\sqrt{v_{K\alpha}} * 10^{-8}$  (v in Hz) for the K<sub>a</sub> lines



**Fig.5.** Moseley's plot: the atomic number vs square root of the frequency  $\left(\frac{v}{10^{16}}\right)$  v in Hz [45]

For other hand, the X-rays fluorescence (XRF) is a process where a material is exposed to X-rays of high energy, and as the X-rays (or photons) strike an atom (or a molecule) in the sample, the energy is absorbed by the atom. If the energy is high enough, a core electron is ejected out of its atomic orbital. Then, an electron from an outer shell drops into the unoccupied orbital to fill the hole left behind. This transition of the electron gives off an X-ray of fixed characteristic energy (X-ray fluorescence) which can be detected by a fluorescence detector.

The energy needed to eject a core electron is characteristic of each element and also the emitted energy by the transition [5], [8], [9], [45]. Therefore, it is possible to know what elements a material is made through the fluorescence of X-rays and by a fluorescence detector.



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Fig.6. The X-ray fluorescence process [45]

## 1.3. Sources of X-rays

## X rays Tube

One form of generating X rays is the stopping of energetic electrons in the electromagnetic field of the atomic nuclei. A high vacuum tube is usually used for it. The unit of primary source 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-rays tube. X-rays are produced when the electrons are suddenly decelerated with a high voltage and directed to the collision with the metal target (anode). The X rays are produced due the fact that accelerated charges give off electromagnetic radiation as Maxwell Theory establishes. These X-rays are commonly called bremsstrahlung or "braking radiation" (white radiation also). Therefore, part of the kinetic energy of the electron is transformed into X-rays (bremsstrahlung) but the bigger part of this energy is transformed into thermal energy of the anode. Then, it must be very heat resistant. Besides, if the bombarding electrons have sufficient energy, they can knock and put out an electron of an inner shell of the atoms of the metal target. Then, the electrons from the higher states drop down to the vacant shell, emitting characteristic (fluorescence) x-rays (photons) with precise energies determined by the energy levels of the electrons. The minimum wavelength  $\lambda$  (in pm), can be derived from the energy E (in keV) o V(in kV), by the relationship:  $\lambda_{min}$ =1239.81/E or  $\lambda_{min}$ =1239.81/V. Ulrey bombarded tungsten targets with electrons of four different energies and obtained the graph of the intensity against the wavelength of the emitted X-rays (for some accelerating voltages) [5], [8], [9], [45].



Fig.7. Scheme of a x-rays tube [45]



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Fig.8. Intensity (y abscissa) versus the wavelength of the X-rays (x abscissa) [45]

The efficiency is low and the intensity grows with the atomic number Z of the anode. The maximum intensity is at  $1.5 \lambda_{min}$ . It is characterized by a continuous distribution of radiation which becomes more intense and shifts toward lower wavelength when the energy of the bombarding electrons is decreased or shifts toward higher frequencies when the energy of the bombarding electrons is increased. The general fall of the x-rays absorption coefficient with the increasing energy of the incident photon is interrupted by a sharp rise when the energy is equal to the binding energy of an electron shell (K, L, M, etc.) of the absorber material. This energy is the minimum energy at which a vacancy can be created in the particular shell and it is referred to as the 'edge' or 'critical excitation' energy. They are generated when an 'initial' vacancy in an inner shell (created by a x-ray or an electron excitation), is filled by another electron transfer from other shell, thus leaving a 'final' vacancy in that shell. The energy of the line is equal to the difference in the binding energies of the shells of the 'initial' and 'final' vacancies. 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 the excitation of the K, L, M, N or O levels. Lines are identified both by the common labels as for example:  $K_{\alpha 1}$ ,  $K_{\alpha 2}$ , etc. or the term labels with the 'initial' and 'final' vacancies as for example: KLIII, KLII, etc. The relationship between the wavelength of a characteristic x-ray photon and the atomic number Z of the excited element was firstly established by Moseley [5], [8], [9], [45]. With the insights from the Bohr model, it is as follows:

$$hv_{K\alpha} = \frac{3}{4}hcR(Z-1)^{2}eV \quad (hcR: Rydberg in unit of energy: 13.6 eV)$$

$$\frac{hc}{\lambda} = \frac{3}{4}hcR(Z-1)^{2}eV \qquad (R = \frac{me^{4}}{8\epsilon_{0}{}^{2}ch^{3}}: Rydberg Constant)$$

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

$$\delta = R(\frac{1}{n'^{2}} - \frac{1}{n^{2}}) \qquad \delta = \frac{3}{4}R \quad \text{for the } K_{\alpha} \text{ lines}$$

$$\frac{1}{\lambda} = \delta(Z-\sigma)^{2} \quad \frac{1}{\sqrt{\lambda}} = \sqrt{\delta} (Z-\sigma)$$

Where,  $\delta$  is a constant which takes different values for each spectral series,  $\sigma$  is the shielding constant which has a value of just less than unity. In the case of a metal with a small atomic number such as copper or molybdenum, we observe very characteristic lines. The characteristic lines are caused by electrons being knocked out of the K shell of an atom and then the electrons from the L shell fill the vacancies in this K shell. The emitted energies in this



process corresponds to the so-called  $K_{\alpha}$  (n=2 to n=1) and  $K_{\beta}$  (n=3 to n=1) lines. For other hand, the transitions to the n=2 or L shell are designated as L x rays. For example, n=3 to n=2 is  $L_{\alpha}$ , n=4 to n=2 is  $L_{\beta}$ , etc.



**Fig.9.** Characteristic x ray peaks from a x rays tube anode (Cu and Mo): Intensity versus wavelength of the X-rays [45]

The continuous distribution of x rays which forms the base for the two sharp peaks is the bremsstrahlung radiation (braking radiation or white radiation). The probability that a vacancy in a given shell will result in the emission of a X-ray is the fluorescence yield of this shell. Not all the vacancies result in the production of characteristic X-ray photons since there is a competing internal rearrangement process known as the Auger effect. The ratio of the 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 [5], [8], [9], [45].

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 1 must change by +/-1, and the J quantum number (where J= 1+ s and s is the spin quantum number) must change by 0 or 1. In effect, it means that for the K series only p, s transitions are allowed, yielding two lines for each principal level change.

Vacancies in the L level follow similar rules and give rise to L series lines. There are more of the L lines since there are more allowed transitions. In practice, the number of observed lines of a given element will depend of the atomic number of the element, the excitation conditions and the wavelength range of the employed spectrometer [5], [8], [9], [45]. While the most of the observed fluorescent lines are normal, certain lines may also occur in the X-ray spectra that do not fit the basic selection rules which are called forbidden lines and they are shown in the center portion of the below figure.

The X-ray spectra are the plot of the reciprocal of the square root of the wavelength as a function of the atomic number, for the K, L and M series:

$$\frac{1}{\sqrt{\lambda}} = \sqrt{\delta} \ (\text{Z-}\sigma) \qquad \delta = R(\frac{1}{n'^2} - \frac{1}{n^2}) \qquad \delta = 3R/4 \quad \text{for the } K_\alpha \text{ lines}$$

A scale in wavelength is also shown to indicate the range of wavelengths over which a given series occurs.





**Fig.10.** Moseley's plot indicating normal and forbidden fluorescent lines: plot of  $\frac{1}{\sqrt{\lambda}}$  versus Z where  $\frac{1}{\sqrt{\lambda}} = \sqrt{\delta}$  (Z- $\sigma$ ) and K= $\sqrt{\delta}$  [45]

#### 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 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 [5], [8], [9], [45]. It is possible to get monoenergetic X-rays photons with the decay product of Am (241) in Np (237) as it is shown in the next figure:



Fig.11. Decay of Am (241) in Np (237) [45]



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## 1.4. X-rays Detector (transducer for converting x-rays photon energy into voltage pulse)

The detectors work through a process of photoionization in which the interaction between the incoming X-ray photon and the active material (detector) produces a number of electrons. The current produced by these electrons is converted to a voltage pulse by a capacitor and a resistor, such that one digital voltage pulse is produced for each incoming X-ray photon. In addition, the detector must be sensitive to the appropriate photon energies, which means that it must be applicable to a given range of wavelengths or energies. There are two other important properties that an ideal detector should possess: proportionality and linearity. Each incoming x-ray photon which enters to the detector produces a voltage pulse, and if the size (amplitude) of the voltage pulse height selection is used. Pulse height selection means rejecting pulses of voltage levels (by using electronics) other than those pulses corresponding to the characteristic lines being measured. For other hand, X-rays enter to the detector at a certain rate and if the output pulses are produced at the same rate, the detector is called linear. Linearity is very important when the various count rates produced by the detector are used as measures of the photon intensity for each measured line [5], [8], [9], [45].

#### 1.5. The proportional gas detector, the avalanche formation

The proportional gas detectors are almost always operated in the pulse mode. It relies on the phenomenon of gas multiplication to amplify the charge represented by the original ion pairs created within the gas. Gas multiplication is a consequence of increasing the electric field within the gas to a sufficient high value. At low values of the field, the electrons and ions created by the incident radiation simply drift to their respective collecting electrodes. During the migration of these charges, many collisions occur with neutral gas molecules. Because of their low mobility, positive or negative ions achieve a very little average energy through the collisions [5], [8], [9], [45].

Free electrons are easily accelerated by the applied field and they have significant kinetic energy when undergoing to this collision. If this energy is greater than the ionization energy of the neutral gas molecule, it is possible to create an additional ion pair in the collision (secondary ionization). Because the average energy of the electron through the collisions increases with the increasing electric field, there is a threshold value of the field above which this secondary ionization will occur. In typical gases and at atmospheric pressure, the threshold field is of the order of  $10^6$  V/m. Also, the electron liberated by this secondary ionization process will be accelerated by the electric field. During its subsequent drift, it undergoes to collisions with other neutral gas molecules and it can create additional ionization [5], [8], [9], [45].

Therefore, the gas multiplication process takes the form of a cascade, known as the Townsend avalanche, in which each free electron created in the collision can potentially create more free electrons by the same process [5], [8], [9], [45]. The fractional increase in the number of electrons per unit path length is governed by the Townsend equation:  $\frac{dn}{n} = \alpha dx$ .

In this equation,  $\alpha$  is called the first Townsend coefficient for the gas. Its value is zero for the electric field values below the threshold and generally increases with the increasing field strength. For a spatially constant field,  $\alpha$  is a



constant in the Townsend equation. The solution of the differential equation establishes that the density of electrons grows exponentially with the distance as the avalanche progresses:  $n(x)=n(0)e^{\alpha x}$ .

For a cylindrical geometry used in most of the proportional counters, the electric field increases in the direction that the avalanche progress. In the proportional counter, the avalanche finishes when all free electrons have been collected at the anode. Under proper conditions, the number of secondary ionization events can be kept proportional to the number of primary ion pairs formed and the total number of ions can be multiplied by a factor of many thousands. The formation of an avalanche involves many energetic collisions electron-atom in which a variety of excited atomic (or molecular) states may be formed [5], [8], [9], [45].

## 1.6. Regions of the Detector Operation

At very low values of the voltage, the field is insufficient to prevent recombination of the original ion pairs, and the collected charge is less than the original collected charge by the original ion pairs. As the voltage is raised, the recombination is suppressed and the region of ion saturation is achieved. This mode is the normal operation mode for ionization chambers. If the voltage is still increased, the threshold field at which the gas multiplication begins is reached. Then, the collected charge begins to multiply, and the pulse amplitude will increase [5], [8], [9], [45].

In some regions of the electric field, the gas multiplication will be linear, and the collected charge will be proportional to the number of original ion pairs created by the incident radiation. It is the region of proportionality and linearity and represents the operation mode of conventional proportional counters and we use the detector in this region [5], [8], [9], [45].

If we increase the applied voltage or the electric field still more, it can introduce nonlinear effects. The most important is related to the positive ions, which are also created in each secondary ionization process. Although the free electrons are quickly collected, the positive ions move much more slowly and during the time that it takes to collect the electrons, they barely move at all. Thus, each pulse within the counter creates a cloud of positive ions, which are very slow to be dispersed as they drift toward the cathode [5], [8], [9], [45].

If the concentration of these ions is sufficiently high, they represent a space charge that can significantly change the shape of the electric field within the detector. Because further gas multiplication is dependent on the magnitude of the electric field, some nonlinearity will begin to be observed. These effects mark the onset of the region of limited proportionality and linearity in which the pulse amplitude still increases with the increasing number of initial ion pairs, but not in a linear form. If the applied voltage is made sufficiently high, the space charge created by the positive ions can become completely dominant to determine the next history of the pulse [5], [8], [9], [45].

Therefore, the avalanche proceeds until a sufficient number of positive ions have been created to reduce the electric field below the point at which an additional gas multiplication can take place [5], [8], [9], [45]. Then, the process is self-limiting and it will finish when the same total number of positive ions have been formed regardless of the number of the initial ion pairs created by the incident radiation. Then, each output pulse from the detector is of the same amplitude and it does not more reflect any property of the incident radiation [5], [8], [9], [45]. This



region is the Geiger Müller region of operation, with lower counting rates, higher voltage and no proportionality. The regions of the detector operation are shown in the next graph:



Fig.12. Regions of the detector operation [45]

## 1.7. Geometry of the detector

The anode consists of a fine wire which is positioned along the axis of a large hollow tube that serves as the cathode. The polarity of the voltage is important because the electrons must be attracted toward the center axial wire [5], [8], [9], [45]. This voltage is essential for two reasons:

1. Gas multiplication requires large values of the electric field. It is given by:  $E(r) = \frac{V}{r} ln(\frac{b}{a})$ 

Where, V is the voltage applied between the anode and the cathode, a is the anode wire radius, b is the cathode inner radius. Therefore, large values of the electric field occur in the immediate vicinity of the anode wire where r is small. As the electrons are attracted to the anode, they are attracted toward the high field region.

2. If uniform multiplication is achieved for all ion pairs formed by the original radiation interaction, the region of gas multiplication is confined to a very small volume compared with the total volume of the gas. Under these conditions, almost all primary ion pairs are formed outside the multiplication region, and the primary electron simply drifts to that region before the multiplication takes place. Therefore, each electron undergoes the same multiplication regardless of its original position of formation, and the multiplication factor wil be the same for all original ion pairs [5], [8], [9], [45].



Fig.13. Cylindrical geometry for the proportional counter [45]



#### 1.8. Absorption in the used detectors

We can see in the next Fig., the absorption efficiency versus the energy for different gases at normal pressure:



Fig.14. Absorption efficiency vs energy for He, Air, N<sub>2</sub>, Ar, Kr and Xe [45]

We use in this experiment as detectors two proportional counters filled with Argon and Xenon. As a quench gas, 3% of CO2 is added to the counting gas. The gamma ray penetrates a 0.01 inch of beryllium window before it enters to the counter. The beryllium window allows the entry of x rays into the detector. For this reason, materials with low atomic number Z are used and the window is thin. Also, the window must support the gas of the detector and it must resist pressure differences. For X rays up to several Angstroms, these conditions are met by thin foils of Al or Be. For lower photon energies, thin organic films are used, because they are fragile and semi-permeable. The cylindrical counter is made of iron. The operation voltage of the counters is: max. 2,0 kV, recommended 1,6 kV for Argon; max. 2,4 kV and recommended 2,0 kV for Xenon. Proportional counters have found several applications in the detection and energy measurement of low energy gamma rays and x-rays in the region up to 100 keV [5], [8], [9], [45].

### 1.9. Measurement of the energy of an incoming photon

The gamma photon is absorbed by the electron of an atom of the gas detector by the photoelectric effect. The photoelectron has the next kinetic energy:  $K=E_{\gamma}-E_{B}$  where  $E_{B}$  is the bound energy of the electron ( $E_{B}=U_{o}$ ). The bound energy is called work function. It is equal to the minimum energy  $E_{\gamma}=hf_{min}$  necessary to eject an electron with kinetic energy almost with zero value:  $E_{\gamma}=E_{B}$   $hf_{min}=E_{B}$   $f_{min}=E_{B}/h$   $E_{B}=$ work function K $\approx 0$  for  $f_{min}$ .

Afterward, the photoelectron loses its kinetic energy by causing further ionization (Bethe-Bloch). The number of ion-electron pairs produced is proportional to the energy of the electron. There is an average energy needed to ionize one atom and it depends on the gas detector used. The atom ionized by the photon has a vacancy in an inner shell and thus it emits a characteristic (fluorescence) X-ray or an Auger electron. But if an auger electron is emitted, then it also causes further ionizations. For other hand, the X-ray photon can make another photoeffect or it can escape. If all energy is spent, then the number of electron-ion pairs is given by:  $n=E_{\gamma}/\epsilon$  where  $\epsilon$  is the average energy needed to ionize one atom in the gas and  $E_{\gamma}$  is the energy of the X-ray photon [5], [8], [9], [45].



We have the recombination process when the voltage is not applied. If the voltage is increased, we have migration of the electrons to the anode wire (small radius). If the voltage is more increased, the electrons win more energy and it causes further ionizations. Therefore, there is an avalanche of electrons, and they soon arrives to the anode wire [5], [8], [9], [45]. The number of electrons arriving at the anode is: N=n\* $\alpha$  where  $\alpha$  is the amplification factor of the inner gas. Thus, N and the pulse height are proportional to E<sub> $\gamma$ </sub>.

## 2. X Rays Diffraction

If we want to describe the interaction between x rays and matter, the following effects should be examined: scattering, generation of secondary radiation, pair production, ionization, luminescence as well as diffraction and refraction. Therefore, it is very important the understanding of the Laue method diffraction. We can see the diffraction effects if the wavelength of the radiation and the measurements of the object on which the radiation will be diffracted, are at the same order of magnitude.

Thus, the measurements of a diffraction lattice have to be of the same scale of the radiation wavelength and typically, ruled grating have some 1000 lines/nm. A lattice of this kind cannot be artificially produced but the atoms of a crystal form the lattice themselves.

Max von Laue, Friedrich and Knipping recorded the first diffraction images of a crystal in the X-ray range. If a crystal is irradiated with polychromatic radiation, this radiation will be diffracted under different angles depending on the wavelength.

As detector, we use the scintillation counter. Therefore, the X rays stimulate the process of luminescence within of the crystal. The optical photons generated in this way hit a photocathode and release electrons in this cathode. These electrons are strengthened through a voltage cascade.

Because the strength of the voltage impulse (size or amplitude) depends on the energy of the X-rays, not only the radiation intensity but also the spectral distribution can be detected (and thus, the elements of which the material is constituted). For the Laue method, position sensitive detectors like the following are necessary to detect the diffracted radiation [47], [48], [49], [50], [51], [52], [53]: Image plates, Photographic film, Multiple wire counters, Fluorescent screens with image intensifiers.

## 2.1. Crystals, Miller indices and Bravais lattices

Firstly, a coordinate system adapted to the symmetry features has to be defined and the point of intersection between the plane and the coordinate system must be described.

For other hand, the position of the atoms in the crystal can be described in terms of the Miller indices. The Miller indices can describe a lattice or surface in a crystal by means of a coordinate system indicating the cutting points of a given surface with the axes of such coordinate system.

There are two forms to describe the meaning of the Miller indices, by a point in the reciprocal lattice or as the inverse intercepts along the lattice vectors  $(a_1, a_2, a_3)$ . Nevertheless, it is necessary to select the three lattice vectors  $a_1$ ,  $a_2$  and  $a_3$  which define the unit cell. Thus, the three primitive reciprocal lattice vectors are determined too  $(b_1, b_2, a_3)$ .



and  $b_3$ ). The reciprocal lattice of a lattice is usually known as Bravais lattice. It is the lattice in which the Fourier transform of the spatial wave function of the direct (original) lattice is represented. In the next figure, we can see a two dimensional crystal in direct space and its reciprocal lattice [47], [48], [49], [50].



Fig.15. Two dimensional crystal in direct space and its reciprocal lattice [31]

For the case of an infinite three-dimensional lattice which is defined by its primitive vectors  $(a_1, a_2, a_3)$ , the reciprocal lattice can be determined by obtaining its three reciprocal primitive vectors, by using the next formulas:

$$b_1 = 2\pi \frac{a_2 x a_3}{a_1 \cdot (a_2 x a_3)}$$
$$b_2 = 2\pi \frac{a_3 x a_1}{a_2 \cdot (a_3 x a_1)}$$
$$b_3 = 2\pi \frac{a_1 x a_2}{a_3 \cdot (a_1 x a_2)}$$

For other hand, the three Miller indices h,k,l establishes planes orthogonal to the reciprocal lattice vector:  $g_{hkl}=h\mathbf{b}_1+k\mathbf{b}_2+l\mathbf{b}_3.$ 

The h,k,l indices indicates a normal to the planes in the basis of the primitive reciprocal lattice vectors. These coordinates h,k,l are integers and the requirement of the lowest terms means that it is the shortest reciprocal lattice vector in the given direction.

For other hand, h,k,l establishes a plane that intercepts the three points  $a_1/h$ ,  $a_2/k$ , and  $a_3/l$  or some multiple. Thus, the Miller indices are proportional to the inverses of the intercepts of the plane, in the basis of the lattice vectors. If one of the indices is zero, it means that the planes do not intersect this axis or it intercepts at the infinity.

If we consider (hkl) planes intersecting one or more lattice points (lattice planes), the perpendicular distance between adjacent lattice planes (d) is related to the shortest reciprocal lattice vector ( $g_{hkl}$ ) orthogonal to the planes by the next formula:  $d = \frac{2\pi}{|g_{hkl}|}$ .

In the next figure, we have planes (shaded plane) with different miller indices in a cubic crystal [47], [48], [49], [50].:



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Fig.16. Planes (shaded plane) with different miller indices in a cubic crystal [31]

In the next figure, we have examples of directions:



Fig.17. Examples of directions [31]

Next figure shows examples to determine indices for a plane using intercepts with axis, left (1 1 1), right (2 2 1).



Fig.18. Examples to determine indices for a plane using the intercepts with the axis, left (1 1 1), right (2 2 1) [31]



We can observe other examples in the next figure:



Fig.19. Different surfaces and Miller indices: (001), (123) and (1 10) [31]

Bravais realized that crystals are not continuously structured but lattice structured. These lattice are regular combinations of small volumes in the form of parallelepipeds whose angles and edge lengths correspond to the axial system of the respective crystal [47], [48], [49], [50]. Therefore, the fundamental element of the crystal is the lattice. The crystal lattice consist of a formation of three lattice vectors which are identical to the axial system and the unit cell as the smallest unit volume of the crystal which includes the symmetry of lattice. For the cubic system, we have the next symmetries: simple or primitive cubic, body centered cubic, face-centered cubic (fcc) Bravais lattices [47], [48], [49], [50]. The choice of the axial system and the unit cell is based on the symmetry of the lattices. The interplanar crystal spacing can be determined with the help of the Miller indices. For the cubic system, it is:  $d(hkl) = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$ .

For example, the Bravais lattice of LiF is face-centred cubic (fcc). The atomic base consists of a lithium atom and a fluoride atom. NaCl also has the symmetry (fcc) as the LiF structure but they differ in the size of lattice parameter a. The Bravais lattice of CsCl is cubic although the atoms seem to form a body centered cubic lattice. The atomic base consists of a Cs and Cl atom [47], [48], [49], [50].





## 2.2. Electron Diffraction (wave character of the electrons)

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 [54].



The electrons emitted by a metallic filament are accelerated through the potential difference  $\Delta V$  and then, they are impinged on a nickel crystal. By applying the law of energy conservation, it is possible to obtain:

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

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

By replacing the values of h, m, e and  $\Delta V=150$  V, the wavelength is  $\lambda=1$  A. A crystal can diffract x-rays with wavelength of 1 A. This diffraction is due to the fact that the crystal contains defined planes which are called Bragg planes where the atoms are located. 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. The Bragg formula is as follows:  $n\lambda=2dsen\theta$ . This formula that is applicable for the light would be also valid for electrons if they also behave as waves. 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.21.** Electron Diffraction: Two electron beams with identical wavelength and phase approach a crystalline solid and scattered of two different atoms. The lower beam traverses and additional length of  $2d\sin\theta$ . Constructive interference occurs when this length is equal to an integer multiple of the wavelength of the radiation

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

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. 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 [54].

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,...

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



## 2.3. Bragg reflection of X rays on crystal

The radiation is only measurable in those directions where the radiation reflection on the parallel atomic planes interferes constructively. The interference condition is given by:

 $n\lambda = 2dsin\theta$ 

Where, n is an integer number,  $\lambda$  is the wavelength, d is the interplanar distance and  $\theta$  is the scattering angle. This equation limits the possible diffraction structures because the three factors have to be correctly chosen. The description in the reciprocal space is the reciprocal lattice. A spatial vector of the reciprocal lattice is:  $\overrightarrow{S_{hkl}} = h\overrightarrow{b_1} + k\overrightarrow{b_2} + l\overrightarrow{b_3}$ 

The (hkl) indices are the Miller indices of any lattice plane within the crystal. This vector  $\overrightarrow{S_{hkl}}$  is perpendicular to the lattice plane and thus, parallel to the normal vector  $\vec{n}$  and its length is reciprocal to the reduced interplanar crystal spacing:

$$\overrightarrow{\mathbf{S}_{hkl}} = \frac{1}{d_{hkl}} \overrightarrow{n_{hkl}}$$
$$\mathbf{d}(hkl) = \frac{d}{n}$$

Thus, also the Bragg equation can be written down in the reciprocal space coordinates (vector form):

 $\overrightarrow{\Delta s} = \overrightarrow{s} - \overrightarrow{s_{o}} = 2\sin\theta \overrightarrow{n_{hkl}} \text{ where } \overrightarrow{n_{hkl}} = d_{hkl} \quad \overrightarrow{S_{hkl}} = \frac{d}{n} \overrightarrow{S_{hkl}}$  $\overrightarrow{\Delta s} = 2\sin\theta \frac{d}{n} \overrightarrow{S_{hkl}} \text{ and } n\lambda = 2dsin\theta$ 

Then, it is obtained:  $\frac{\overrightarrow{\Delta s}}{\lambda} = \overrightarrow{S_{hkl}}$ 



Fig.22. Cross section of a 3-D Ewald construction [31]



In the Ewald construction, we have that:

- a) the interference condition is fulfilled for one reciprocal lattice point.
- b) the interference condition is fulfilled for none of the reciprocal lattice points.

The vector  $\vec{s_0}$  of the direction of the primary ray is drawn in the points of the reciprocal lattice and thus, the vector points to the lattice point. Then, a sphere with the radius  $1/\lambda$  is drawn around the origin of  $\vec{s_0}$ . If the sphere intersects a further lattice point, the interference condition is fulfilled and the connecting distance of both lattice points is equal to the scattering vector s, which is equal to 1/d where d is the interplanar distance [47], [48], [49], [50]..

## 2.4. Symmetry elements, point group of symmetry

The symmetry elements listed in the symbol of the point groups are also called generating symmetry elements [47], [48], [49], [50]. In the cubic system, the point group m3m is the generating symmetry elements which generate three four-fold axes parallel to (100) and 12 two fold axes parallel to (110) as well as a symmetry centered and three fold axes along (111).

#### 32 Crystalline punctual groups

 Table 1. Crystalline punctual groups [31]

Crystal system	Crystal class	Symmetry elements	Degree of symmetry	Laue classes (center of symmetry)	Piezo - pyro
m	ī	ī	2	Yes	No
Triclinic	1	1	1	No	Pyro
	2/m	2/m	4	Yes	No
Monoclinic	2	2	2	No	Pyro
	m	m	2	No	Руго
Ortho	mmm	2/m2/m 2/m	8	Yes	No
Ortilo-	222	222	4	No	Piezo
rnombic	mm2	mm2	4	No	Pyro
	4/mmm	4/m2/m 2/m	16	Yes	No
	422	422	8	No	Piezo
	4mm	4mm	8	No	Pyro
Tetragonal	$\overline{4} 2m$	$\overline{4}$ 2m	8	No	Piezo
	4/m	4/m	8	Yes	No
	4	4	4	No	Pyro
	4	4	4	No	Piezo
Trigonal	<u>3</u> m	32m	12	Yes	No
	32	32	6	No	Piezo
	3m	3m	6	No	Pyro
	3	3	6	Yes	No
	3	3	3	No	Pyro
	6/mmm	6/m2/m 2/m	24	Yes	No
	622	622	12	No	Piezo
	6mm	6mm	12	No	Pyro
Hexagonal	$\overline{6}$ 2m	<u>6</u> 2m	12	No	Piezo
	6/m	6/m	12	Yes	No
	6	6	6	No	Pyro
	$\overline{6}$	$\overline{6}$	6	No	Piezo
	m3m	4/m 3 2/m	48	Yes	No
	432	432	24	No	No
Cubic	$\overline{4}3m$	$\overline{4}3m$	24	No	Piezo
	m 3	2/m 3	24	Yes	No
	23	23	12	No	Piezo



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2.5. Fourteen Bravais Lattices



Fig.23. Fourteen Bravais Lattices [31]

## 2.6. Crystalline Systems Bravais

 Table 2. Crystalline Systems Bravais [31]

Name	Number of Bravais lattices	© Bart Van Zeghbroeck 2007 <b>Conditions</b>	Primitive	Base- centered	Body- centered	Face- centered
Triclinic	1	$a_1 \neq a_2 \neq a_3$ , $\alpha \neq \beta \neq \gamma$	√			
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ , $\alpha = \beta = 90^\circ \neq \gamma$	√	√		
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ , $\alpha = \beta = \gamma = 90^\circ$	√	√	√	√
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^{\circ}$	~		✓	
Cubic	3	$a_1 = a_2 = a_3$ , $\alpha = \beta = \gamma = 90^{\circ}$	✓		√	√
Trigonal	1	$a_1 = a_2 = a_3$ , $\alpha = \beta = \gamma < 120^\circ \neq 90^\circ$	√			
Hexagonal	1	$a_1 = a_2 \neq a_3$ , $\alpha = \beta = 90^\circ$ , $\gamma = 120^\circ$	✓			



## 2.7. Stereogram of the 32 crystalline punctual groups





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Fig.24. Stereogram of the 32 crystalline punctual groups [31]

## 2.8. Brillouin Zone

We can see the reciprocal lattices (dots) and the corresponding first brillouin zone.



Fig.25. Brillouin Zone [31]



## 2.9. Cubic System lattice



Fig.26. Cubic System lattice [31]

2.10. Real Space (primitive direct lattice  $a_1$ ,  $a_2$  or a, b) & Reciprocal Space (reciprocal lattice  $b_1$ ,  $b_2$  or  $a^*$ ,  $b^*$ )



Fig.27. Real Space and Reciprocal Space [54]





#### RECIPROCAL LATTICE OF FCC IS BCC



Fig.29. Reciprocal lattice of FCC: BCC [31]



## 2.11. The Laue experiment of X ray diffraction on crystal

When the X rays interact with the crystals, they can be diffracted by the lattices of the crystals. This diffraction happens if the spectrum of the incoming X-ray field has energies big enough so the photons can interact with the lattices of the crystal. If we want to see X-ray diffraction, the object or crystal to be analyzed must have diffracting lattice plane distances of the same order of the X-rays wavelength. It is similar just like the diffraction of visible light. Then, the crystal will diffract the X rays in different angles.

The incident X rays interact with the electrons of the atoms within the crystal. After the interaction, secondary radiation is produced. It must have special conditions for the wave trains of the secondary radiation to superpose in constructive ways. It is why the interference conditions are similar to the ones in the optical range. The lattice planes of the monocrystal orientated towards the collimated primary ray "choose" the wavelength from the X-ray spectrum according to the Bragg equation. The constructive interference patterns are registered with a space resolving plane detector. Therefore, we get a projection of the lattice planes of a crystal (**Laue diagram**) on the detector which reflects the symmetry characteristics of the crystal to a certain degree (**Laue Symmetry**) [47], [48], [49], [50].

## 2.12. Scintillators and Photomultipliers





The scintillator counter consists of a scintillator sheet, light guide, photomultiplier and the electronics at the photomultiplier base to read out the signal. The scintillator is composed of three components: primary scintillator, the wavelength shifter and the base material.

There are inorganic scintillator (such as sodium iodide) and organic (such as a plastic like polystyrene). The charge particles pass through the material and excite electrons. They can de-excite emitting a photon. The primary scintillation light is emitted in the ultraviolet (UV) range preferentially. This photon would be exactly of the correct energy to be reabsorbed by the material and the scintillator is not transparent to its own scintillation light. For this reason, the light is transferred to a wavelength shifter which absorbs the UV light and reemits it at a longer wavelength (green). It reduces the energy of the photon and so, the photon emitted is of longer wavelength with not enough energy to be reabsorbed. The scintillator sheet is highly polished, and light is conducted by total internal reflection. In this way, the emitted light can get out of the scintillator. The light must be transmitted from the scintillator to a sensor of the photomultiplier. It is done by a light guide and then, it can be detected by the photomultiplier. The emitted light from the wavelength shifter is matched with the spectral sensitivity of the photomultiplier by this light guide.



Besides, the primary scintillator and the wavelength shifter are mixed with organic material in a plastic scintillator to form a polymerizing structure. At the liquid scintillators the 2 components are mixed with an organic base. We need about 100 eV to produce one photon in a organic scintillator.

The photomultiplier converts the optical signal to an electrical signal and provides a high amplification.



Fig.31. The photomultiplier [31]

The photomultiplier consists of an evacuated glass envelope coated at one end with a photocathode made of alkali metals, which is maintained at a large negative potential. The photons liberate electrons (by photoelectric effect) from the cathode, which are accelerated towards a (less negative) dynode, and knock out a number of secondary electrons.

This process continues until a large signal is collected at the anode. The typical gain of the photomultiplier is of the order of  $10^7$  and normally a pulse of a few mV per detected photon is produced.

Finally, the connections to the photomultiplier are made through the photomultiplier base, which contains a chain of resistors to provide the correct voltages for the dynodes and cathode [51], [52], [53].

## 2.13. Experimental set up



Fig.32. Main components of the experimental set up [31]

We can observe the X-ray tube with metallic coat, a two circle goniometer (measure the angles between the faces of the crystal) with crystal mounting and the crystal to be examined as well as an image intensifier for the transformation of the X-ray reflexes into visible light. Then, the Laue diffraction images can be registered and analyzed with the help of a CCD-camera and a computer [47], [48], [49], [50], [51], [52], [53].

## 2.14. Thought Experiments (Gedankenexperiment)

## Which symmetry elements are important for Laue group m3m?

(100), (110) and (111). It generate three four-fold axes parallel to (100), 4 threefold axes parallel to (111) and 12



two-fold axes parallel to (110) as well as a symmetry centered [47], [48], [49], [50].

# Show the symmetry elements of the cube with rotation axes and mirror planes for the Surfaces (100), (110), (111).

The rotation axes and the mirror planes are the following:

## **Rotation axes:**



Fig.33. Rotation axes [31]

## Mirror planes:





Fig.34. Mirror planes [31]

## With what indices are these m3m symmetry elements described?

The mirror planes are described by the following indices:

For the first set of mirror planes, it is for <100>, we have:



**Fig.35.** Set of mirror planes for <100> [31]



For the second set of mirror planes, it is for <110>, we have:



**Fig.36.** Set of mirror planes for <110> [31]

## Which is the angle between the planes (100) and (110); (100) and (111); (110) and (111)?.

First case: By applying the point product between the normal vectors (miller indices):  $1 = \sqrt{1} \sqrt{2} \cos(\theta)$ , we find the angle is 45 °.

Second case: By applying the same point producto:  $1 = \sqrt{1} \sqrt{3} \cos(\theta)$  we find the angle is 54,7°.

Third case: By applying the same point product:  $2 = \sqrt{2} \sqrt{3} \cos(\theta)$  we find the angle is 35, 26°.

## Which are the diffraction images with each four fold and a two fold symmetry by rotating the crystal module in the Java applet?

## 4- Fold Symmetry





 $\rho = 90^{\circ}$ 

 $\rho = 0^{\circ}$ 

Fig.37. 4-Fold Symmetry (Diffraction) [31]

## 2-Fold Symmetry:



 $\rho$  =135 °

Fig.38. 2-Fold Symmetry [31]



 $\rho$  =45 °



Assign the correct sample term to the suggested answers in Fig.

For  $\rho = 0^{\circ}$  and  $\phi = 0^{\circ}$ 



Fig.39. Diffraction images and Sample Solutions [31]



**Sample a: Solution 3**. We can see a square like pattern, only that in this case it looks rotated. The front plane of solution 3 is a <100> (for  $\rho = 0$  and  $\phi = 0$ ), so the pattern should be square. The rotation in the Laue pattern can be explained because of the lateral plane being a <110>

**Sample b: Solution 2**. In this case, we have that the front plane is a <110>, it is like if the cube was rotated an angle  $\rho = 45^{\circ}$ . We would then expect a symmetric Laue pattern like showing one border of the cube in the middle of the Laue pattern and the two external borders at the sides of the pattern

**Sample c: Solution 1**. The front plane is a <100> just like the lateral and upper planes. For this reason, we can see immediately the form of a square (for  $\rho = 0$  and  $\phi = 0$ ) in the Laue diffraction pattern

## 3. Diffraction and Interference for the electron by using the Fourier Approach and Wave Properties

## 3.1. 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:  $\Delta p \Delta x \ge \frac{(\frac{h}{2\pi})}{2}$  where p is the momentum,



x is the position of the particle and h is the Planck constant. 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:

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

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

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

$$\Delta E \Delta t = v \Delta p \frac{\Delta x}{v} = \Delta p \Delta x \ge \frac{(\frac{h}{2\pi})}{2} \qquad \Delta E \Delta t \ge \frac{(\frac{h}{2\pi})}{2}$$

This principle is also a support for the modern quantum mechanics and for the Schrodinger's Quantum Theory, 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 2 $\theta$ . Thus, the results of the interaction cannot be predicted [9]. The x component of the momentum of the photon can vary from +psen $\theta$  to -psen $\theta$ :

## $\Delta p_x \approx 2psen\theta = 2\frac{h}{\lambda}sen\theta$

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:



 $\Delta p_x \approx 2 \frac{h}{\lambda} \operatorname{sen} \theta$ . It is necessary to use a light with a lower energy, (lower frequency or larger wavelength) or a microscope with a smaller angle  $\theta$  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:

$$\operatorname{sen}\theta = 1.28 \frac{\lambda}{D} \qquad \operatorname{sen}\theta \approx \frac{\lambda}{D} \quad D \approx \frac{\lambda}{\operatorname{sen}\theta}$$

Where, D is the linear separation of the points of the object that are solvable in the image:  $D=\Delta x \quad \Delta x = \frac{\lambda}{\sin\theta}$ 



Fig.40. Experiment imagined by Bohr for the Uncertainty Principle

The photon is scattered somewhere within the resolvable limits of the microscope D. This also corresponds to the uncertainty in the location of the electron  $\Delta x=D$ . If we want to reduce the localization range  $\Delta x$ , a light with a higher energy, higher frequency or smaller wavelength or a microscope with a higher resolution angle  $\theta$  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:  $\Delta p_x \Delta x = 2 \frac{h}{\lambda} \operatorname{sen} \theta \frac{\lambda}{\operatorname{sen} \theta}$ 

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

Besides, 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 Heisenberg. Other 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.41. Electron diffraction by a slit for the Uncertainty Principle



The Fig 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:  $\frac{a}{2} \operatorname{sen} \theta = m \frac{\lambda}{2}$ .

It is possible to observe at the Fig., that there is a minimum, if the path defence 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: asen $\theta$ = $\lambda$  where a is the slit width: a= $\Delta x$  sen $\theta$ = $\lambda/a$  sen $\theta$ = $\lambda/\Delta x$ .

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  $a >> \lambda$  there is no the diffraction pattern. The diffraction pattern appears when  $a \le \lambda$ . If we want to reduce the uncertainty of the position ( $\Delta x$ ), 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 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  $\Delta p_x$  is given by  $\Delta p_x=2p_x$ (maximum uncertainty of the x component of the momentum: from  $-p_x$  to  $+p_x$ ):  $sen\theta \approx \theta = \frac{p_x}{p} = p_x = p_x = h/\lambda$ 

$$p_{x} = \frac{h}{\lambda} sen\theta$$
  
$$\Delta p_{x} = 2p_{x} \qquad \Delta p_{x} = 2\frac{h}{\lambda} sen\theta$$

 $\Delta p_x \Delta x = 2 \frac{h}{\lambda} \operatorname{sen} \theta \Delta x$   $a = \Delta x$   $\operatorname{sen} \theta = \lambda / \Delta x$  (first minimum)

 $\begin{array}{ll} \Delta p_{x} \Delta x = 2\frac{h}{\lambda} \frac{\lambda}{\Delta x} \Delta x & \Delta p_{x} \Delta x = 2h > \frac{(\frac{h}{2\pi})}{2} \\ \Delta p_{x} \Delta x > \frac{(\frac{h}{2\pi})}{2} & \text{Uncertainty Principle of Heisenberg} \end{array}$ 

Besides, if the arrival of the electrons is 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 with two slits and the result is known as the Copenhagen Interpretation. Then, 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 position. On the contrary, if we want to reduce the uncertainty in the position, 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].



## 3.2. Diffraction: Fourier Approach

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

 $f(x,t)=F_{o}$   $-x_{o}/2 \le x \le x_{o}/2$ 

f(x,t)=0  $x>x_0/2$  or  $x<-x_0/2$ 



Fig.42. Constant energy radiation for the light

The Fourier integral at the domain of the angular frequency w is given by the next function:  $F(w) = F[f(x,t)] = \int_{-\infty}^{\infty} f(x,t)e^{-jwt}dt$ 

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

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

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

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

$$F(w) = \frac{F_0}{-jw} (-2j \operatorname{sen} \frac{wx_0}{2}) \qquad e^{-jwt} = \cos(wt) - j\operatorname{sen}(wt)$$
(wyve)

 $F(w) = \frac{2F_0}{w} \operatorname{sen}\left(\frac{wx_0}{2}\right) = F_0 x_0 \frac{\operatorname{sen}\left(\frac{wx_0}{2}\right)}{w\frac{x_0}{2}}$ 

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



**Fig.43**. 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:

 $f(x,t)=F_o+F_ocos(w_ot) -x_o/2 \le x \le x_o/2 \qquad x_o \le \lambda_o \text{ (to produce diffraction)}$ 

f(x,t)=0  $x>x_0/2$  or  $x<-x_0/2$ 

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



Fig.44. 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  $F(\omega) = F[f(t)]$  the Fourier integral of  $f(t)\cos \omega_0 t$  is as follows:

$$F[f(t)e^{j\omega_{0}t}] = F(\omega - \omega_{0}) \qquad \cos(\omega_{0}t) = \frac{1}{2}[e^{j\omega_{0}t} + e^{-j\omega_{0}t}]$$

$$F[f(t)\cos(\omega_{0}t)] = F\left[f(t)\frac{1}{2}[e^{j\omega_{0}t} + e^{-j\omega_{0}t}]\right] = \frac{1}{2}F[f(t)e^{j\omega_{0}t}] + \frac{1}{2}F[f(t)e^{-j\omega_{0}t}]$$

$$= \frac{1}{2}F(\omega - \omega_{0}) + \frac{1}{2}F(\omega + \omega_{0})$$

$$f(x,t)=F_{0} - x_{0}/2 \le x \le x_{0}/2$$

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

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

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

$$\frac{1}{2}F(\omega - \omega_0) + \frac{1}{2}F(\omega + \omega_0) = \frac{F_0 \operatorname{sen}(\frac{x_0}{2}(w - w_0)}{w - w_0} + \frac{F_0 \operatorname{sen}(\frac{x_0}{2}(w + w_0)}{w + w_0}$$

$$f(x,t)=F_0 + F_0 \operatorname{cos}(w_0 t) \quad -x_0/2 \leq x \leq x_0/2 \quad x_0 \leq \lambda_0 \text{ (to produce diffraction)}$$

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

$$F(w) = \frac{2F_0}{w} \operatorname{sen}\frac{wx_0}{2} + \frac{F_0 \operatorname{sen}(\frac{x_0}{2}(w - w_0)}{w - w_0} + \frac{F_0 \operatorname{sen}(\frac{x_0}{2}(w + w_0)}{w + w_0}$$

$$F(w) = \frac{1}{w} \operatorname{sen}(\frac{wx_0}{2}) + \frac{w-w_0}{w-w_0} + \frac{w+w_0}{w+w_0}$$
$$F(w) = F_0 x_0 \frac{\operatorname{sen}(\frac{wx_0}{2})}{w\frac{x_0}{2}} + \frac{F_0 \frac{x_0}{2} \operatorname{sen}(\frac{x_0}{2}(w-w_0))}{\frac{x_0}{2}(w-w_0)} + \frac{F_0 \frac{x_0}{2} \operatorname{sen}(\frac{x_0}{2}(w+w_0))}{\frac{x_0}{2}(w+w_0)}$$

+ --

The magnitude of the spectrum  $|F(\omega)|$  para x<sub>0</sub>=2, w<sub>0</sub>=0.1 and F<sub>0</sub>=7 is showed in the next figure:



**Fig.45.** Spectrum  $|F(\omega)|$  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].

## 3.3. 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. Gaussian

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 image 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  $\Delta t_{rms} = \sigma$ . It is possible to calculate the inflexion points as follows:

$$f(t) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}} \qquad \qquad \frac{df}{dt} = \frac{-t}{\sigma^3\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}}$$
$$\frac{d^2f}{dt^2} = \frac{t^2}{\sigma^5\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}} - \frac{1}{\sigma^3\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}} \qquad \qquad \frac{t^2}{\sigma^5\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}} - \frac{1}{\sigma^3\sqrt{2\pi}} e^{-\frac{t^2}{2\sigma^2}} = 0$$
$$t^2 = \sigma^2 \qquad t = \pm \sigma$$
$$\Delta t_{\rm rms} = \sigma \quad \text{For } \sigma = 2 \quad \Delta t_{\rm rms} = 2$$



**Fig.46.** Graph of the Gaussian Distribution for  $\sigma=2$ 

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

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

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

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

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

$$t^2 + 2j\sigma^2wt = (t + j\sigma^2w)^2 - (\sigma^2jw)^2$$

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

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

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

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

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

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

$$F(w) = \frac{e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} \qquad \frac{dF}{dw} = -\frac{\sigma^2 w e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}}$$
$$\frac{d^2 F}{dw^2} = \frac{\sigma^4 w^2 e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} - \frac{\sigma^2 e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} \qquad \frac{\sigma^4 w^2 e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} - \frac{\sigma^2 e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} = 0$$
$$\sigma^4 w^2 = \sigma^2$$



**Fig.47.** Graph of the Fourier Integral of the Gaussian Distribution for  $\sigma=2$ 

In w= $\pm 0.5$ , F''(w)=0, then the rms deviatio  $\Delta w_{rms}=0.5$  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  $\sigma$ .

In Physic terms, it means that if the time is increased or stretched (more  $\Delta t$ ), then it implies a decrease or narrowed (less  $\Delta w$ ) 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  $\Delta x$ ), then it implies a decrease or narrowed (less  $\Delta k$ ) 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 w=
$$2\pi f$$
 f=w/( $2\pi$ ) E= $\frac{h}{2\pi}w$   
p=h/ $\lambda$  k= $2\pi/\lambda$   $\lambda$ = $2\pi/k$  p= $\frac{h}{2\pi}k$ 

The formula are as follows:

$$\Delta w \Delta t = 1 \qquad E = \frac{h}{2\pi} w \qquad \frac{h}{2\pi} \Delta w \Delta t = \frac{h}{2\pi} \qquad \Delta E \Delta t = \frac{h}{2\pi}$$
$$\Delta k \Delta x = 1 \qquad p = \frac{h}{2\pi} k \qquad \frac{h}{2\pi} \Delta k \Delta x = \frac{h}{2\pi} \qquad \Delta p \Delta x = \frac{h}{2\pi}$$

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  $\frac{1}{\sigma\sqrt{2}}$ .

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



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$$\frac{dg}{dt} = \frac{-2t}{\sigma^4 2\pi} e^{-\frac{t^2}{\sigma^2}} \qquad \frac{d^2g}{dt^2} = \frac{4t^2}{\sigma^6 2\pi} e^{-\frac{t^2}{\sigma^2}} - \frac{2}{\sigma^4 2\pi} e^{-\frac{t^2}{\sigma^2}}$$
$$t^2 = \frac{\sigma^2}{2} \qquad t = \pm \frac{\sigma}{\sqrt{2}} \qquad \Delta t_{\rm rms} = \frac{\sigma}{\sqrt{2}}$$

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

$$F(w) = \frac{e^{-\frac{\sigma^2 w^2}{2}}}{\sqrt{2\pi}} \qquad |F(w)|^2 = h(w) = \frac{1}{2\pi} e^{-\sigma^2 w^2}$$
$$\frac{dh}{dw} = -\frac{2\sigma^2 w e^{-\sigma^2 w^2}}{2\pi} \qquad \frac{d^2 F}{dw^2} = \frac{4\sigma^4 w^2 e^{-\sigma^2 w^2}}{2\pi} - \frac{2\sigma^2 e^{-\sigma^2 w^2}}{2\pi}$$
$$\frac{4\sigma^4 w^2 e^{-\sigma^2 w^2}}{2\pi} - \frac{2\sigma^2 e^{-\sigma^2 w^2}}{2\pi} = 0$$
$$4\sigma^4 w^2 = 2\sigma^2 \qquad w^2 = \frac{1}{2\sigma^2}$$
$$w = \pm \frac{1}{\sqrt{2}\sigma} \qquad \Delta w_{\rm rms} = \frac{1}{\sigma\sqrt{2}}$$

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

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

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

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

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

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.

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

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

$$\Delta E \Delta t \ge \frac{\frac{h}{2\pi}}{2} \qquad \Delta p \Delta x \ge \frac{\frac{h}{2\pi}}{2}$$

## 3.4. 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].

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.



Fig.48. Double Slit Experiment with the intensity pattern on the screen detector

If  $\varphi_A$  and  $\varphi_B$  (wave functions for each slit) are different wave function for the electron. They are solutions of the Schröndiger Equation. Besides, they represent a possible state for the electron [5]. Then, the superposition of the two waves is also solution of the Schröndiger 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  $\varphi$  is a probabilistic wave function

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

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

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 Schröndiger Approach. Besides, this



probabilistic behaviour is used at the Schröndiger 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  $\varphi$ . The wave serves to the electron as guide during the interference process. The electrons from the wave  $\varphi_A$  or  $\varphi_B$  after the slits are positioned in a new guide wave  $\varphi$  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.

## 3.5. 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 Schröndiger 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.

## 3.6. 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  $\varphi_A$  or  $\varphi_B$  after the slits are positioned in a new guide wave  $\varphi$  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.

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

 $E^2 = p^2 c^2 + m_o^2 c^4$  Relativistic Dirac equation For light  $m_o=0$ 

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

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

p=mv momentum for a particle

 $mv = \frac{h}{\lambda}$   $\lambda = \frac{h}{mv}$  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 Schröndiger 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... [4], [5], [9].



Fig.49. 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<sup>2</sup>) at the stationary level with  $m = \frac{h}{\lambda v}$  where  $\lambda$  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<sup>2</sup>. As consequence of it, the wavelength  $\lambda$  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,...) 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 occurs 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.

#### 4. Variant Mass of the Electron at the atom

#### 4.1. 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 Sommerfeld Model has established [19], [20], [21], [22], [23], [24]. The nucleus is at the focus of the ellipse as the sun in one focus at the Planetary System [19], [20], [21], [22], [23], [25], [26]. There is a strong analogy between the Planetary System and the Atom System at this model.



Fig.50. 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. Respect to the gravitational energy emission, it is demonstrated by theory, experiment and result the discovery formula which describe exactly the variant mass of a particle which emits gravitational energy which was demonstrated by myself at the article: The Fundament of the Mass and Effects of the Gravitation on a Particle and Light in the mass, time, distance, velocity, frequency, wavelength: Variant Mass for a Particle which emits Gravitational Energy for a particle orbiting a large Planet or Sun and for a Binary Star and Variant Frequency for the Light passing close a Gravitational Field from a Massive Object (Sun). The result of the emission of the total gravitational energy (bond total energy) for a particle orbiting a large Planet or Sun and for a Binary Star.

At the atom, 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.

## 4.2. Formula development of the total mass of the electron at the electric potential of the nucleus and quantization formula

$$c^2 dm = \frac{dp}{dt}ds + \frac{ke^2}{R^2}dR$$
  $c^2 dm = vdp + \frac{ke^2}{R^2}dR$   $v=ds/dt$ 

p=mv m=p/v The electrical force is equal to the centrifugal force:

$$\begin{split} \frac{ke^2}{R^2} &= m \frac{v^2}{R} & \frac{ke^2}{R^2} = \frac{pv}{R} \\ \frac{ke^2}{R} &= pv & -\frac{ke^2}{R^2} dR = pdv + vdp \\ \frac{ke^2}{R^2} dR &= -pdv - vdp & c^2 d(\frac{p}{v}) = vdp - pdv - vdp \\ c^2 d(\frac{p}{v}) &= -pdv & c^2 \frac{vdp - pdv}{v^2} = -pdv \\ -c^2 \frac{dp}{v} &= p(1 - \frac{c^2}{v^2}) dv & -c^2 \frac{dp}{p} = v(1 - \frac{c^2}{v^2}) dv \\ ln \frac{p}{p_o} &= -((\frac{v^2 - v_o^2}{2c^2}) - (ln v - lnv_o)) \\ \frac{p}{p_o} &= \frac{v}{v_o} e^{-(\frac{v^2 - v_o^2}{2c^2})} & p = mv \quad p_o = m_o v_o \\ \frac{mv}{m_o v_o} &= \frac{v}{v_o} e^{-(\frac{v^2 - v_o^2}{2c^2})} & \text{total relativistic mass of the electron at the atom} \end{split}$$

 $\Delta m = m_0 c^2 - mc^2 = m_0 c^2 (1 - e^{-\left(\frac{v^2 - v_0^2}{2c^2}\right)}) \text{ total decrease mass of the electron at the atom}$ 

If  $v^2 \ll c^2$ , then it is obtained for the classical case:

$$e^{-\left(\frac{v^2 - v_0^2}{2c^2}\right)^2} = 1 - \left(\frac{v^2 - v_0^2}{2c^2}\right) + \frac{\left(\frac{v^2 - v_0^2}{2c^2}\right)^2}{2!} + \cdots$$

$$\frac{\left(\frac{v^2 - v_0^2}{2c^2}\right)^2}{2!} \text{ and other terms are neglected}$$

$$\frac{ke^2}{R^2} = m\frac{v^2}{R} \qquad \frac{ke^2}{mR} = v^2 \qquad m = m_0(1 - \left(\frac{v^2 - v_0^2}{2c^2}\right))$$

$$\left(\frac{v^2 - v_0^2}{2c^2}\right) = \frac{ke^2}{2m_0c^2}\left(\frac{1}{R} - \frac{1}{R_0}\right) \qquad R_f = R \qquad R_i = R_0$$

$$m = m_0 (1 - \frac{ke^2}{2m_0c^2} (\frac{1}{R} - \frac{1}{R_0}))$$
 mass of the electron: classical approach



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 $m_0c^2 - mc^2 = \frac{ke^2}{2}(\frac{1}{R} - \frac{1}{R_0})$  total decrease mass: classical approach

 $m_o c^2 - mc^2 = \frac{ke^2}{2R}$  total decrease mass of the electron: classical approach (R<sub>o</sub>->∞)

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:

$$\begin{split} & E = mc^2 - m_0 c^2 \qquad m = m_0 e^{-(\frac{v^2 - v_0^2}{2c^2})} \\ & E = m_0 c^2 (e^{-\left(\frac{v^2 - v_0^2}{2c^2}\right)} - 1) \quad \text{total relativistic energy for the electron in the atom} \\ & \text{If } v^2 << c^2, \text{ then it is obtained for the classic case:} \\ & e^{-\left(\frac{v^2 - v_0^2}{2c^2}\right)} = 1 - \left(\frac{v^2 - v_0^2}{2c^2}\right) + \frac{\left(\frac{v^2 - v_0^2}{2c^2}\right)^2}{2!} + \cdots \\ & \left(\frac{\left(\frac{v^2 - v_0^2}{2c^2}\right)^2}{2!}\right)^2 \text{ and other terms are neglected} \\ & E = -m_0 \left(\frac{v^2 - v_0^2}{2}\right) \quad \text{classical approach} \\ & \frac{ke^2}{R^2} = m \frac{v^2}{R} \qquad \frac{ke^2}{mR} = v^2 \qquad \left(\frac{v^2 - v_0^2}{2}\right) = \frac{ke^2}{2m_0} \left(\frac{1}{R} - \frac{1}{R_0}\right) \\ & E = -m_0 \left(\frac{ke^2}{2m_0} \left(\frac{1}{R} - \frac{1}{R_0}\right)\right) \qquad E = -\left(\frac{ke^2}{2R}\right) \quad \text{total energy for the electron at the atom or bound energy} \end{split}$$

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  $R_f < R_i \quad \Delta E = E_f - E_i = \left(-\frac{ke^2}{2R_f}\right) - \left(-\frac{ke^2}{2R_i}\right)$  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  $R_f > R_i \Delta E$  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  $E_f$ )

$$\Delta E = -\left(\frac{ke^2}{2}\left(\frac{1}{R_i} - \frac{1}{R_f}\right)\right) \qquad \Delta E = \left(\frac{ke^2}{2}\left(\frac{1}{R} - \frac{1}{R_o}\right)\right) \qquad R_i = R_o \qquad R_f = R_o$$

The formula of Balmer Series is as follows:

$$\frac{1}{\lambda} = R_y (\frac{1}{n'^2} - \frac{1}{n^2}) \quad n > n' \quad R_y = 1.099731 \times 10^7 \text{ m}^{-1}: \quad R_y = \frac{\text{me}^4}{8\varepsilon_0^2 \text{ ch}^3} \text{ Rydberg Constant}$$
$$\frac{f}{c} = R_y (\frac{1}{n'^2} - \frac{1}{n^2}) \quad f = cR_y (\frac{1}{n'^2} - \frac{1}{n^2}) \quad f = \frac{\text{me}^4}{8\varepsilon_0^2 \text{ h}^3} (\frac{1}{n'^2} - \frac{1}{n^2}) \qquad \lambda = c/f$$

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:

$$\Delta E = hf = \frac{mhe^4}{8\epsilon_0{}^2h^3} \left(\frac{1}{n'^2} - \frac{1}{n^2}\right) \qquad \Delta E = \frac{me^4}{8\epsilon_0{}^2h^2} \left(\frac{1}{n'^2} - \frac{1}{n^2}\right)$$

This formula can be compared with the mass formula development for the classic approach:  $\Delta E = \left(\frac{ke^2}{2}\left(\frac{1}{R} - \frac{1}{R_0}\right)\right)$ 

$$\frac{me^4}{8{\epsilon_0}^2h^2}(\frac{1}{n'^2} - \frac{1}{n^2}) = \left(\frac{ke^2}{2}(\frac{1}{R} - \frac{1}{R_0})\right)$$

n: main quantum number of the initial state with radius  $R_o$ 

n': main quantum number of the final state with radius R

$$\frac{e^2}{4\pi\varepsilon_0(2)(\frac{\varepsilon_0h^2}{\pi m e^2})} \left(\frac{1}{n'^2} - \frac{1}{n^2}\right) = \left(\frac{ke^2}{2}\left(\frac{1}{R} - \frac{1}{R_0}\right)\right) \qquad k=1/(4\pi\varepsilon_0)$$
$$\frac{ke^2}{2}\left(\frac{1}{(\frac{\varepsilon_0h^2}{\pi m e^2})n'^2} - \frac{1}{(\frac{\varepsilon_0h^2}{\pi m e^2})n^2}\right) = \left(\frac{ke^2}{2}\left(\frac{1}{R} - \frac{1}{R_0}\right)\right)$$

It is concluded that the radius must be proportional to the number  $n^2$ .

$$R = a_{o} n^{2} \quad R_{o} = a_{o} n^{2}$$

$$R = a_{o} n^{2} \quad a_{o} = \frac{\varepsilon_{o} h^{2}}{\pi m e^{2}} \quad a_{o} = 0,529 \times 10^{-10} \text{ m} = 0,529 \text{ A} \qquad \text{Bohr radius}$$



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:  $R = \frac{\epsilon_0 h^2}{\pi m e^2} n^2$ .

The Constant of Rydberg is obtained as follows:

$$f = cR_y(\frac{1}{n'^2} - \frac{1}{n^2}) \qquad \Delta E = hf = chR_y(\frac{1}{n'^2} - \frac{1}{n^2}) \quad \Delta E = \left(\frac{ke^2}{2a_0}\left(\frac{1}{n'^2} - \frac{1}{n^2}\right)\right)$$

 $\operatorname{ch} R_y \left( \frac{1}{n'^2} - \frac{1}{n^2} \right) = \left( \frac{\operatorname{ke}^2}{2a_0} \left( \frac{1}{n'^2} - \frac{1}{n^2} \right) \right) \qquad \operatorname{ch} R_y = \frac{\operatorname{ke}^2}{2a_0}$ 

$$R_{y} = \frac{ke^{2}}{2cha_{o}}$$
 h: Planck Constant  $a_{o} = \frac{\varepsilon_{o}h^{2}}{\pi me^{2}}$   $k=1/(4\pi\varepsilon_{o})$  c: light velocity  

$$R_{y} = \frac{me^{4}}{8\varepsilon_{o}^{2}ch^{3}}$$
  $R_{y} = 1.0997313414*10^{7} \text{ m}^{-1}$  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:

$$chR_{y} = \frac{ke^{2}}{2a_{o}} \qquad h = \frac{ke^{2}}{2a_{o}cR} \qquad a_{o} = \frac{\varepsilon_{o}h^{2}}{\pi me^{2}}$$
$$k=1/(4\pi\varepsilon_{o})=9*10^{9} \text{ N m}^{2}/\text{C}^{2} \qquad \varepsilon_{o}: \text{ vacuum permittivity}=8,85*10^{-12} \text{ Farad/m}$$

a<sub>o</sub>: Bohr radius=5,3  $*10^{-11}$  m c: light velocity=3 $*10^8$  m/s

e: electron charge= $1,6*10^{-19}$  Coulomb (C)

 $R_y = 1.097313414 \times 10^7 \text{ m}^{-1}$ : Rydberg Constant

By using those values, it is possible to obtain the Planck Constant:

h=6,63\*10<sup>-34</sup> J-s Planck Constant

## 4.3. 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 [24], [27], [28], [29], [30] are as follows:

$$v = \frac{Ze^2}{2\epsilon_0 nh} \quad r = \frac{n^2h^2\epsilon_0}{\pi m_0 Ze^2} \quad E = \frac{-z^2e^4m_0}{8\epsilon_0^2h^2n^2}$$

Z: atomic number of the atom e: charge of the electron

 $\epsilon_o$ : 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:

## Table 3. Physical constants

h	6,63*10 <sup>-34</sup> J-s
εο	8,85*10 <sup>-12</sup> Farad/m
π	3,1416
mo	9,11*10-31 kg
e	1,6*10 <sup>-19</sup> C
r <sub>o</sub>	0,528 <b>Å</b>

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 and 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:  $(m_o-m)c^2=hf=K$ 

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:  $mc^2=m_oc^2-hf$ 

$$mc^2 = 511875 - 13,6 = 511861,4 eV$$

For other hand, the mass electron calculation with the mass development formula is as follows:

$$m = m_0 e^{-(\frac{v^2}{2c^2})}$$

The velocity is given by this formula:

$$v = \frac{Ze^2}{2\varepsilon_0 nh}$$

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,  $\varepsilon_0$ , 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 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 the 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<sup>2</sup>=511875-3,4

For other hand, the mass electron calculation with the mass development formula is as follows:

$$m = m_0 e^{-(\frac{v^2}{2c^2})}$$

The velocity is given by this formula:

$$v = \frac{Ze^2}{2\epsilon_o nh}$$

By replacing the values for Z (Z=1), e,  $\varepsilon_0$ , n (n=2), h, it is obtained:

v=1090744,859 m/s

By replacing this value at the mass formula, it is achieved:

mc<sup>2</sup>=511871,6 eV

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  $(mc^2=m_oc^2-hf)$  and for the formula of the variant mass for the electron at the atom after the energy emission:  $m = m_o e^{-(\frac{v^2}{2c^2})}$ . 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.

n	v	r	E=hf Ecinetica (ionization energy)	mc <sup>2</sup> =m <sub>o</sub> c <sup>2</sup> -hf	$m = m_o e^{-(\frac{v^2}{2c^2})}$
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



#### **Bound of Diatomic Molecules**

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



Fig.51. Center of mass for diatomic molecules

mr=MR R=(m/M)r r'=r+R r'= r+(m/M)r  
r'=
$$\frac{M+m}{M}$$
r r= $\frac{M}{M+m}$ r'  
m $\frac{v^2}{r} = \frac{kZe^2}{r'^2}$   
 $v^2 = r\frac{kZe^2}{mr'^2} = \frac{M}{M+m}r'\frac{kZe^2}{mr'^2} = \frac{kZe^2}{2m_o r'}$  M=m=m<sub>o</sub>  
 $v = \sqrt{k\frac{Ze^2}{2m_o r'}}$ 

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:  $m_0 = 1,67353 * 10^{-27}$  kg.

The nuclear separation is:  $r=0.74 \text{ A} (1 \text{ A}=10^{-10} \text{ m}).$ 

$$v = \sqrt{k \frac{Ze^2}{2m_o r}} k = \frac{1}{4\pi\epsilon_o} = 9*10^9 \text{ Nm}^2/\text{C}^2 Z = 1 e = 1.6*10^{-19} \text{ C}$$

v=30499, 52739 m/s

$$m = m_0 e^{-(\frac{v^2}{2c^2})}$$
 where c is the light velocity c=3\*10<sup>8</sup> m/s.

$$\Delta mc^{2} = (m_{o}e^{-(\frac{v^{2}}{2c^{2}})})c^{2} - m_{o}c^{2}$$

$$\Delta mc^{2} = 4.8648 \text{ eV}$$

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:  $\, m_o {=} 1,67353 \, \, {*}10^{\, {-}27} \, kg.$ 

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  $H_2$ .



$$v = \sqrt{k \frac{Ze^2}{2m_o r}} k = \frac{1}{4\pi\epsilon_o} = 9*10^9 \text{ Nm}^2/\text{C}^2 Z = 1 e = 1.6*10^{-19} \text{ C}$$

v=23851,53228 m/s

$$m = m_0 e^{-(\frac{v^2}{2c^2})}$$
 where c is the light velocity  $c=3*10^8$  m/s

 $\Delta mc^2 = (m_0 e^{-(\frac{v^2}{2c^2})})c^2 - m_0 c^2$ 

 $\Delta mc^2 = 2,9752064 \text{ eV}$ 

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 / 2 A).

For the  $O_2$ , it is obtained:

The mass of  $O_2$  is:  $m_0=2,77 * 10^{-26}$  kg.

The nuclear separation is:  $r=1.21 \text{ A} (1 \text{ A}=10^{-10} \text{ m}).$ 

v = 
$$\sqrt{k \frac{Ze^2}{2m_o r}}$$
 k= $\frac{1}{4\pi\epsilon_o}$ =9\*10<sup>9</sup> Nm<sup>2</sup>/C<sup>2</sup> Z=1 e=1,6\*10<sup>-19</sup> C

v=5862,6459,81 m/s

$$m = m_0 e^{-\left(\frac{v^2}{2c^2}\right)}$$

Where, c is the light velocity  $c=3*10^8$  m/s

 $\Delta mc^2 = (m_o e^{-(\frac{v^2}{2c^2})})c^2 - m_o c^2$ 

 $\Delta mc^2 = 2,9752083 \text{ eV}$ 

It is possible to calculate the rotation frequency w for the  $O_2$ :

$$L = Iw \approx \frac{h}{2\pi}$$
$$w \approx \frac{h}{2\pi I}$$

 $I=2m_o(r/2)^2=2,0277*10^{-46} \text{ kg m}^2$ 

By replacing the value of the Planck constant h, it is obtained:

w=5,20\*10<sup>11</sup> 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.



## 4.4. Conclusions

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 [24], [27], [31], [32], [33], [34]. 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 [22], [23], [26]. 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 [22]. 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.

Bohr proposed a model with some postulates to solve the instability of 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 Schröndiger Theory (wave probabilistic theory) and Heisenberg Theory (matrix theory) [22], [23]. The duality wave-particle of De Broglie and the Heisenberg Uncertainty Principle were support for the development of the modern quantum physics. The stationary states or levels correspond to those functions which satisfy the Schröndiger Equation [22], [23]. The electron in an atom no excited (electron in a stationary level) is at rest. Thus, it cannot radiate energy because it corresponds to a stationary level of the atom [22], [23]. At this research, it is to demonstrate the discovery formula which describes exactly the variant mass of a charged particle as the electron at the atom which emits electromagnetic energy from one stationary level to other: Variant mass of the electron at the Atom. 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.

## 5. The Variant Mass for an accelerated charged particle

## 5.1. Introduction

Firstly, it is demonstrated by theory, calculations and results the discovered formula which describe the mass of an accelerated charged particle emitting electromagnetic radiation. Finally, thought experiments, experimental tests and calculations are presented which confirm the formula theoretically demonstrated.



## 5.2. Formula Development: Variant Mass for an accelerated charged particle

An accelerated charged particle emits electromagnetic radiation and then, the mass decreases [35],[36], [37]. This electromagnetic radiation emitted is the Maxwell radiation for an accelerated charged particle.

It is applied the energy conservation for the development of the formula for the mass of the particle.

The change of the kinetic energy of the particle dK is transformed in an decreasing of the relativistic mass-energy  $dE=c^2dm$  (by using the famous formula for the energy-mass for every particle:  $E=mc^2$ ). Thus, it is obtained:

 $-c^2 dm = dK$ 

$$dK = dW = Fds = \left(\frac{dp}{dt}\right)ds = dp\left(\frac{ds}{dt}\right) = d(mv)v = v^2dm + mvdv$$

 $-c^2dm = v^2dm + mvdv$ 

 $-c^2 dm = v^2 dm + mv dv$ 

 $(-c^2 - v^2)dm = mvdv$ 

 $\frac{dm}{m} = \frac{v}{(-c^2 - v^2)} dv$ 

By doing the respective integration, it is obtained:

 $\int_{m_{o}}^{m} \frac{dm}{m} = \int_{0}^{v} -\frac{2v}{2(c^{2}+v^{2})} dv$ 

By doing a variable change:  $u=c^2+v^2$ , du=2vdv, it is achieved:

$$\int_{m_o}^{m} \frac{dm}{m} = \int_{c^2}^{c^2 + v^2} - \frac{du}{2u}$$
$$\ln(m) - \ln(m_o) = (-1/2) [\ln(c^2 + v^2) - \ln(c^2)]$$

 $\ln(m/m_0) = \ln[(c^2 + v^2)/c^2]^{-1/2}$ 

 $\ln(m/m_0) = \ln[(c + v)/c]$ 

 $m/m_o = [(c^2+v^2)/c^2]^{-1/2}$ 

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

which is the formula for the mass of an accelerated charged particle which emits electromagnetic radiation.

The kinetic formula is obtained as follows:

$$-c^2 dm = dK$$

and by doing the integration:

 $-mc^2+m_oc^2=K$ , then  $mc^2=m_oc^2-K$   $E=m_oc^2-K$  which is the formula for the kinetic energy:  $K=m_oc^2-mc^2$ 

$$K = m_o c^2 \left(1 - \frac{1}{\sqrt{(1 + \frac{v^2}{c^2})}}\right) \qquad K = m_o c^2 \left(1 - \left(1 + \frac{v^2}{c^2}\right)^{-1/2}\right)$$



For very low velocities, it is obtained:

$$(1 + \frac{v^2}{c^2})^{-1/2} = 1 - \frac{1}{2}\frac{v^2}{c^2} + \frac{3}{8}\frac{v^4}{c^4} + \dots$$
$$K = m_o c^2 (1 - 1 + \frac{1}{2}\frac{v^2}{c^2} - \frac{3}{8}\frac{v^4}{c^4} + \dots)$$

 $\frac{3}{8}\frac{v^4}{c^4}$  and other terms are neglected for very low velocities.

 $K = \frac{1}{2}m_o v^2$  (for very low velocities as the classic formula).

For higher velocities (when v is approaching to  $\infty$ ), the kinetic energy has a maximum value of  $m_0c^2$ , which correspond to the rest mass of the particle. It is completely emitted as electromagnetic radiation at higher velocities.

 $K=m_0c^2-mc^2$ 

 $K \approx m_o c^2 m \approx 0$  (when  $v \approx \infty$ ), almost all energy is emitted as electromagnetic radiation.





It is because the particle is losing mass (due to the emission of electromagnetic radiation) during the movement and therefore, it is possible to get each time more velocity without limit. The kinetic energy has a maximum value of  $m_0c^2$  (0,511 MeV/c<sup>2</sup>) when v is approaching to  $\infty$ .

With respect to the mass formula, it is possible to obtain the next conclusion:

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

Where,  $m_0$  is the mass at rest of the particle.

At this formula, when the velocity v is increasing, the mass m is decreasing too until v is very high ( $\infty$ ) and the value of mass is very low (approximately to 0).

At this point, almost all the mass is emitted (transformed) as electromagnetic energy. Thus, the velocity v can get values higher than the light velocity because of the decreasing mass. The lost mass is equivalent to the mass-energy of the electromagnetic radiation emitted.



f(x)=0.511/(1+(x)<sup>2</sup>)<sup>0.5</sup>



**Fig.53.** Graph of the mass (y axis) (MeV/c<sup>2</sup>) versus the rate v/c (x axis) for an accelerated charged particle. The initial value of the mass is  $0,511 \text{ MeV/c}^2$ 

### 5.3. Thought Experiment (Gedankenexperiment)

### **Thought Experiment (Gedankenexperiment 1)**

\* A rectangular tube of mass M and length L is at rest in a system S. A pulse of electromagnetic radiation of energy E is emitted from one extreme of the tube, and then it is absorbed at the other extreme [38]. In this thought experiment, it is demonstrated as follows that the inertia associated with this radiation is  $m = E / c^2$ .



**Fig.54.** Emission of the electromagnetic radiation pulse (in A) within of the tube of length L. The tube recoils due to the emission of the pulse (momentum conservation). The pulse reaches B and then leaves the tube

Firstly, it is used momentum conservation and then energy conservation as a second form to demonstrate that the inertia associated with this radiation is  $m = E / c^2$ .

#### **Momentum Conservation**

The electromagnetic radiation pulse is emitted to the right. From Maxwell's theory of electromagnetism it is known that an impulse p = E/c is associated with this radiation. In order to preserve the momentum (amount of



movement), the tube moves back to the left with velocity v. If m represents the mass associated with the radiated energy, then the mass of the receding tube is M-m and the conservation of momentum in S requires:

$$(M-m)v = \frac{E}{c}$$
  $v = \frac{E}{(M-m)c}$ 

(p=E/c: impulse of the photon or electromagnetic radiation pulse)

The flight time of the electromagnetic radiation pulse whose velocity is c, is t=(L-x)/c (where x is the displacement of the tube to the left due to the inertia: recoil of the tube). This time is equal to the recoil time of the tube, t=x/v. Combining these times, it is obtained:

$$\frac{(L-x)}{c} = \frac{x}{v}$$
$$\frac{v}{c} = \frac{x}{(L-x)}$$

By replacing the value of v, it is obtained:

$$\frac{E}{(M-m)c^2} = \frac{x}{(L-x)}$$

Since all forces are internal, the center of mass of the system does not change during the emission and absorption processes. If m is the effective mass emitted by radiation, the center of mass will not change if:

Mx=mL

Demonstration:

M(L)=(M-m)(L+x)+mx

 $ML \!\!=\!\! ML \!\!+\!\! Mx \!\!-\!\! mL \!\!-\!\! mx \!\!+\!\! mx$ 

Mx=mL

$$m = \frac{Mx}{L} \quad x = \frac{mL}{M}$$
$$\frac{E}{(M-m)c^2} = \frac{x}{(L-x)}$$

By solving for x, it is achieved:  $x = \frac{EL}{(M-m)c^2+E}$ 

And also: 
$$x = \frac{mL}{M}$$

By equating both equations and solving for m, it is obtained:

$$\frac{EL}{(M-m)c^2+E} = \frac{mL}{M}$$
$$m^2 - \left(\frac{E}{c^2} + M\right)m + \frac{ME}{c^2} = 0$$

There are two mathematical solutions:  $m=E/c^2$  and m=M, but the second solution is not valid because  $m\neq M$ .



Thus, it has been shown that the electromagnetic radiation pulse has an associated mass  $m = E /c^2$  (which previously in the case of the tube belonged to the tube (it is the lost mass in the tube) and was emitted as electromagnetic radiation).

It is possible to get a very important conclusion [38], [39], [40]:

How does the message of moving to the left arrives to the right extreme of the tube after the left extreme of the tube goes back?.

This message of moving to the left for the right extreme of the tube must travel much faster than the light velocity to win the pulse emitted. If the tube were to move like a rigid body the message would travel at infinite velocity. The entire tube does not go back rigidly.

So, this appears that the message of mass lost in the tube m (mass-energy emitted as a pulse of electromagnetic energy travelling at the light velocity) is transmitted along the tube at infinite velocity. This is in accordance with the mass formula for a charged particle that emits electromagnetic radiation because the particle loses approximately all its mass at very high speeds and when v approaches infinity the mass approaches zero. In other words, this lost mass in the tube is related to the infinite transmission of the message along the tube (the lost mass is transmitted along the tube at infinite velocity).

## **Energy Conservation**

 $mc^2=pc$  The energy of the photon emitted is E=pc and m is the lost mass of the tube and emitted as electromagnetic radiation.

M-m is the mass of the tube after the emission of the electromagnetic pulse.

E=hf (energy of the photon)

E=hc/ $\lambda$  (c=  $\lambda$ f for the light velocity)

 $p=h/\lambda$  (for a photon)

Therefore, E=pc for a photon.

Also, it is possible to obtain the same from the Dirac equation:

$$E^2 = m^2 c^4 + p^2 c^2$$

As the mass of the photon is m=0, then, it is obtained E=pc

Thus, the energy of the lost mass of the tube is equal to the energy of the photon emitted:

Therefore: p=mc and because the energy of the photon is E=pc, it is obtained:

 $E=mc^2$  and the associated mass of the photon emitted is  $m=E/c^2$ , where E is the energy of the photon and m is the lost mass on the tube and also the associated mass-energy of the photon emitted.



## **Thought Experiment (Gedankenexperiment 2)**

\* Consider a body B at rest in system S. Two pulses of radiation, each one with E/2 energy, are emitted from B, one pulse moving in the positive x direction and the other in the negative x direction. These pulses are emitted by B, whose energy then decreases by a quantity E and E/2 is the energy of each pulse emitted. For reasons of symmetry, B must remain at rest in S. Now, let us consider the same process with respect to S', which moves with a constant velocity v with respect to S in the negative direction of y. In this case, B moves with velocity v in the positive direction of y'. The radiation pulses are partly directed upward, forming an angle  $\alpha$  with the x' axis. The velocity of B remains constant in S' (after the emission of the radiation) since B remains at rest in S during this process.



**Fig.55.** The body B is at rest in S. Then two pulses of radiation are emitted in the directions shown by the arrows. In S' that moves with respect to S with velocity v in the negative direction of y, the body B moves with velocity v along + y' and the pulses are directed making an angle  $\alpha$  with the x-axis

Now, let's apply the law of momentum conservation in the process in S'. The momentum of B in S' before the emission is Mv (from classic mechanics) along the positive direction of y'. In other words, before the emission takes place, the y' component of the impulse of B is: Mv

After the emission, the body B has mass M' and the momentum is M'v along the positive direction y'. Each radiation pulse emitted has an energy of E/2 and a momentum p=E/2c (p = E/c from classic electromagnetism) with the components of momentum being equal to (E/2c) sin  $\alpha$ .

Therefore, by applying momentum conservation after the emission, it is obtained:

M'v+2(E/2c)sin  $\alpha$ 

By equating the components y' of the impulse before the absorption with those of after absorption, it is achieved:

 $Mv = M'v + 2(E/2c)sin \alpha$ 

 $\sin\alpha \approx \alpha = v/c$  ( v<<c) (classic absorption)



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Mv = M'v + 2(E/2c)(v/c)

$$M=M'+(E/c^2)$$

 $M-M'=E/c^2$ 

Therefore, the decrease in mass  $\Delta M=M-M'$  of the body B is linked to the energy E of the two photons emitted (summed energy) (this energy is also the lost energy of the body B). Therefore:

$$E=(M-M')c^2$$

 $E=\Delta Mc^2$ 

 $\Delta M = E/c^2$  and the associated mass of the photon emitted is  $\Delta M = E/c^2$ , where E is the energy of the photon emitted and  $\Delta M$  is also the lost mass on the body B.

## 5.4. Experimental Test

Every experiment where it is possible to measure the kinetic energy for an accelerated charged particle emitting electromagnetic radiation can be a test for the formula:

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

In fact, a signal or prove of this formula is the maximum kinetic energy of the accelerated charged particle that can be measured. It is  $m_o c^2$  if there is not additional energy given to the particle at the beginning. This energy can be measured at the PMT (photomultiplier) as the maximum kinetic energy for an electron for example.

Also, it is an intrinsic characteristic of the charged particle and independent of the experimental configuration or material used as detector at the experiment for example.

This maximum kinetic energy for the electron appears in the experiment of muons and neutral kaons from ultra dense hydrogen by lepton pair production [39].

At this experiment, we have the next decays:

$$\mu \pm \rightarrow N(e^+ + e^-)$$

 $\mu \pm \rightarrow \mu \pm + N(e^+ + e^-) + KE$  KE: 10-100 MeV dissipation

 $\mu \pm \rightarrow e \pm + neutrinos + N(e^+ + e^-) + KE KE < 105 MeV dissipation$ 

The energy for the pair-production is derived from the kinetic energy of the muons of 10-100 MeV and from the decay of the muons at 105 MeV. As the dissipation energy is around 100 MeV and each pair production process dissipates around 2.04 eV, then we have around 50 lepton pair per muon [39].

The kinetic energy given to the electron-positron pairs increases until that energy is equal to 2x511 keV when a new pair can be produced and energy above this limit gives a new lepton pair [39]. Therefore, at the beginning the electron has a energy equals to the rest mass of the particle.



The accelerated electron has many interactions with the atoms and nuclei of the material used as detector but nevertheless the maximum kinetic energy measured at the PMT is approximately 511 keV [39]. It is the radiated energy for the electron during the path. Also, the same electron energy distribution is found for all materials used as converters [39]. Thus, it depends of an electron property and no of the converter material used [39]. It is in accordance with the kinetic formula for the electron which we have demonstrated before.

It is an intrinsic property of the electron: the way that the electron radiates the energy, specifically the electrodynamic mass. Just the high energy cut-off is close to the rest mass of the electron 511 keV, which is a confirmation of the nature of electron when it shares the electromagnetic radiation. Therefore, the kinetic energy of leptons entering and measured at the PMT is approximately 511 keV (zero-signal cut-off above 511 keV [39]) which is in agreement with the formula demonstrated.

## 5.5. Hydrogen atom: Emission of electromagnetic radiation for the electron at the atom

In order to test the mass formula for an accelerated charged 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[40], [41], [42], [43], [44] are as follows:

$$v = \frac{Ze^2}{2\varepsilon_0 nh}$$

$$r = \frac{n^2 h^2 \varepsilon_o}{\pi m_o Z e^2}$$

$$E = \frac{-z^2 e^4 m_o}{8\varepsilon_o^2 h^2 n^2}$$

- Z: atomic number of the atom
- e: charge of the electron
- $\epsilon_o$ : vacuum permittivity
- n: main quantum number, electron energy level, orbit of the electron
- h: Planck constant

m<sub>o</sub>: rest mass of the electron

Values of constants:

$$Z=1$$

h=6,63\*10<sup>-34</sup> J-s

 $\epsilon_o \!\!=\!\! 8,\!85{}^{*}10^{\text{-}12} \text{ Farad/m}$ 

π=3,1416

 $m_0 = 9,11*10^{-31} \text{ kg}$ 

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e=1,6\*10<sup>-19</sup> C

 $r_0=0,528 \ \dot{A}$  Bohr radius, radius for the first level of the Hydrogen atom

 $1 \dot{A} = 10^{-10} \text{m}$ 

Table 5. Table of physical constants

h	6,63*10 <sup>-34</sup> J-s
εο	8,85*10 <sup>-12</sup> Farad/m
π	3,1416
mo	9,11*10-31 kg
e	1,6*10 <sup>-19</sup> C
r <sub>o</sub>	0,528 <b>Å</b>

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 and 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:

E=hf: energy of the photon emitted (electromagnetic radiation).

It is in coincidence with the formula for the kinetic energy for an Accelerated Charged Particle.

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:

 $mc^2 = m_o c^2$ -hf

mc<sup>2</sup>=511875-13,6 =511861,4 eV

The mass electron calculation with the mass formula for an accelerated charged particle is as follows:

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



The velocity is given by this formula:

$$v = \frac{Ze^2}{2\varepsilon_o nh}$$

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,  $\varepsilon_0$ , n (n=1), h, it is obtained:

v=2181489,72 m/s

By replacing this value at the mass formula, it is achieved:

$$mc^2 = \frac{m_o c^2}{\sqrt{1 + \frac{v^2}{c^2}}}$$

 $mc^2$ =511861,4 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 the 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:

 $mc^2 = m_o c^2 - hf$ 

mc<sup>2</sup>=511875-3,4

=511871,6 eV

For other hand, the mass electron calculation with the mass formula for an accelerated charged particle is as follows:

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

The velocity is given by this formula:

$$v = \frac{Ze^2}{2\varepsilon_o nh}$$

By replacing the values for Z (Z=1), e,  $\varepsilon_0$ , n (n=2), h, it is obtained:

v=1090744,859 m/s

By replacing this value at the mass formula, it is achieved:

$$mc^2 = \frac{m_o c^2}{\sqrt{1 + \frac{v^2}{c^2}}}$$



mc<sup>2</sup>=511871,6 eV 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<sup>2</sup>=m<sub>o</sub>c<sup>2</sup>-hf) and for the formula of the variant mass for an accelerated charged particle:  $mc^2 = \frac{m_o c^2}{\sqrt{1+\frac{v^2}{2}}}$ . 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.

**Table 6.** 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 formula of the variant mass for an accelerated charged particle

n	v	r	E=hf (ionizatin energy)	$mc^2 = m_o c^2 - hf$	$mc^{2} = \frac{m_{o}c^{2}}{\sqrt{1 + \frac{v^{2}}{c^{2}}}}$
1	2181489,719	5,30961E-11	-13,54798602	511861,452	511861,4674
2	1090744,859	2,12384E-10	-3,386996504	511871,613	511871,6168
3	727163,2396	4,77865E-10	-1,50533178	511873,4947	511873,4963
4	545372,4297	8,49537E-10	-0,846749126	511874,1533	511874,1542
5	436297,9438	1,3274E-09	-0,541919441	511874,4581	511874,4587
6	363581,6198	1,91146E-09	-0,376332945	511874,6237	511874,6241
7	311641,3884	2,60171E-09	-0,276489511	511874,7235	511874,7238

## 5.6. Power energy emitted for an Accelerated Charged Particle

The kinetic formula for an accelerated charged particle is as follows:

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

 $K = m_0 c^2 (1 - \frac{1}{\sqrt{(1 + \frac{v^2}{c^2})}})$ 

 $\frac{dK}{dt} = -c^2 \frac{dm}{dt}$  (the change in the kinetic energy of the particle causes a proportional change in its mass, the minus sign is due to the mass decreases)

$$K = m_o c^2 (1 - (1 + \frac{v^2}{c^2})^{-1/2})$$

By doing the respective derivation, it is obtained:

P=dk/dt

 $\frac{dK}{dt} = \frac{m_o v}{(1 + \frac{v^2}{c^2})^{3/2}} \frac{dv}{dt}$ 

$$P = \frac{m_o v}{(1 + \frac{v^2}{c^2})^{3/2}} a$$
 (formula of the power energy for an accelerated charged particle)

The term in parenthesis can be expressed as follows:

$$\left(1+\frac{v^2}{c^2}\right)^{-\frac{3}{2}} = 1 - \frac{3}{2}\frac{v^2}{c^2} + \frac{15}{8}\frac{v^4}{c^4} - \cdots$$

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For v<<c, it is achieved:

$$P = m_o v a \left(1 - \frac{3}{2} \frac{v^2}{c^2}\right)$$
 for very low velocities

If this formula is compared with the Larmor formula (which is used to calculate the power radiated by a non-relativistic point accelerated charge, electromagnetic theory [41], [42], [43], [44]):

$$P = \frac{q^2 a^2}{6\pi\varepsilon_0 c^3} \text{ or in CGS units: } P = \frac{2q^2 a^2}{3c^3}$$
$$\frac{q^2 a^2}{6\pi\varepsilon_0 c^3} = m_0 v \left(1 - \frac{3}{2} \frac{v^2}{c^2}\right) a$$

 $a = \frac{6\pi\varepsilon_0 c^3}{q^2} m_0 v \left(1 - \frac{3}{2} \frac{v^2}{c^2}\right)$  where q is the charge of the particle.

Or if it is used the equivalent formula:

$$P = \frac{2}{3} \frac{m_o r_e a^2}{c}, \text{ it is obtained:}$$

$$\frac{2}{3} \frac{m_o r_e a^2}{c} = m_o v \left(1 - \frac{3}{2} \frac{v^2}{c^2}\right) a$$

$$a = \frac{3vc}{2r_e} \left(1 - \frac{3}{2} \frac{v^2}{c^2}\right) \text{ where } r_e \text{ is the classic electron radius: } r_e = 2,82 \times 10^{-15} \text{ m}$$

#### 5.7. Conclusions

The kinetic formula represents the emission of the electromagnetic radiation for an accelerated charged particle. It is:

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

 $K=m_oc^2-mc^2$ 

K=hf (it corresponds to the ionization energy at the atom of Hydrogen or the energy of the photon emitted or the electromagnetic radiation emitted by the accelerated charged particle).For higher velocities (when v is approaching to  $\infty$ ), the kinetic energy has a maximum value of  $m_o c^2$ , which correspond to the rest mass of the particle. It is completely emitted as electromagnetic radiation at higher velocities.

The mass of the particle after the emission of the electromagnetic radiation (losing the respective mass-energy of the electromagnetic radiation and equal to the lost mass of the particle) is:

$$m = \frac{m_o}{\sqrt{1 + \frac{v^2}{c^2}}}$$
 (mass of the particle after the emission of the electromagnetic radiation)

$$m = \frac{m_o c^2}{\sqrt{1 + \frac{v^2}{c^2}}}/c^2$$
 (mass of the particle in units of energy: eV/c<sup>2</sup>)

Also, it is equals to:



 $mc^2=m_oc^2$ - (hf) where hf is the energy of the photon emitted or emission of the energy of the electromagnetic radiation.

At the mass formula, when the velocity v is increasing, the mass m is decreasing too until v is very high ( $\infty$ ) and the value of mass is very low (approximately to 0). At this point, almost all the mass is emitted as electromagnetic energy. Thus, the velocity v can get values higher than the light velocity because of the decreasing mass. The lost mass is equivalent to the mass-energy of the electromagnetic radiation.

These formulas have been verified by means of theory, thought experiments, experiments and in the hydrogen atom. The formula of the power energy for an accelerated charged particle is as follows:

$$P = \frac{m_o v}{(1 + \frac{v^2}{c^2})^{3/2}} a$$

For very low velocities, it is as follows:

$$P = m_o v a \left( 1 - \frac{3}{2} \frac{v^2}{c^2} \right)$$

The acceleration for very low velocities is as follows:

$$a = \frac{6\pi\varepsilon_0 c^3}{q^2} m_0 v \left(1 - \frac{3}{2} \frac{v^2}{c^2}\right)$$
 where q is the charge of the particle

(or):

$$a = \frac{3vc}{2r_e} \left(1 - \frac{3}{2} \frac{v^2}{c^2}\right)$$
 where  $r_e$  is the classic electron radius.

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