

## Relativistic theory of one- and two electron systems: valley of stability in the helium-like ions

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**Abstract.** A semi-relativistic total energy of the hydrogen-like ions is presented. The established expression taking only into account the dependence of the mass electron on the speed could be considered as a first correction of the Bohr's semi-classical formula. Comparison with relativistic total energy expression obtained from the Dirac's relativistic wave equation is made. In addition, the present relativistic theory of the hydrogen-like ions is extended to the helium isoelectronic series. It is shown that, for the ground state of two electron systems, the relativistic screening constant  $\sigma^{\text{rel}}$  decreases when increasing the nuclear charge up to  $Z=5$ . Beyond,  $\sigma^{\text{rel}}$  increases when increasing  $Z$  and, the plot  $\sigma^{\text{rel}}=f(Z)$  is like a valley of stability where the bottom is occupied by the  $B^{3+}$ -helium-like ion. As a result, only He,  $Li^+$ ,  $Be^{2+}$  and  $B^{3+}$  exist in the natural matter in low temperature. All the other helium-like positive-ions, such as  $C^{4+}$ ,  $N^{5+}$ ,  $O^{6+}$ ,  $F^{7+}$ ,  $Ne^{8+}$ , ..., can only exist in hot laboratory and astrophysical plasmas.

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**Key words:** screening constant, hydrogen-like ions, helium-like ions, valley of stability

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## 1 Introduction

In the year 1913, Bohr managed to explain the spectrum of the hydrogen atom by an extension of Rutherford's planetary atomic model (1911). In the Bohr's model, the negatively charged electron revolves about the positively charged atomic nucleus because of the attractive electrostatic force according to Coulomb's law. On the basis of this classical atomic model, Bohr expresses total energy of the hydrogen atom considering the mass electron as constant, independent then with his velocity. But, since 1905, Einstein develops the theory of relativity and shows that mass of rapid elementary particles varies with their speed. As classical theory is not the framework for interpreting atoms, relativistic corrections of Bohr's formula may be

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done just after 1913. But, these relativistic corrections have been done only in the year 1916 by Sommerfeld (in the framework of the elliptical orbits model) and after in the year 1926 by use of the relativistic wave equation established by Dirac after the discovery of the spin electron (1925) by Uhlenberg and Goudsmith. However, it would be very interesting to make relativistic correction of the Bohr's semi-classical formula before 1916, considering only the dependence of the mass electron on the electron's speed as explained by Einstein. This would permit to interpret theoretically experimental studies who indicate that [1], due to the variation of the mass electron with the speed, the relativistic total energy levels of the hydrogen atom are lowest than the non perturbed total energy levels. Taking after into account the spin electron, one may explain clearly the contribution of the spin in the relativistic effects on the hydrogen-like ions energy-levels. This paper is prepared in the intention to show that, the relativistic effects due to the variation of the electron mass with the speed on the hydrogen isoelectronic sequence energy levels can be put into evidence separately with that due to the spin. In the Dirac's theory, this separation is not possible, as his relativistic wave equation is constructed by considering simultaneously the spin electron and the variation of the mass electron with the speed. In addition, the presented relativistic theory of the hydrogen-like ions is extended to the helium isoelectronic series. It is shown that, for the ground state of two electron systems, the relativistic screening constant  $\sigma^{\text{rel}}$  decreases when increasing the nuclear charge up to  $Z = 5$ .

Beyond,  $\sigma^{\text{rel}}$  increases when increasing  $Z$ , and the plot  $\sigma^{\text{rel}} = f(Z)$  is like a valley of stability where the bottom is occupied by the  $B^{3+}$ -helium-like ion. As a result, only He,  $Li^+$ ,  $Be^{2+}$  and  $B^{3+}$  exist in the natural matter in low temperature ( $LiO$ ,  $Be(OH)_2$ , and  $B_2O_3$  for example). All the other helium-like positive-ions, such as  $C^{4+}$ ,  $N^{5+}$ ,  $O^{6+}$ ,  $F^{7+}$ ,  $Ne^{8+}$ , ..., can only exist in hot laboratory and astrophysical plasmas.

## 2 Theory

### 2.1 Bohr's semi-classical expression of hydrogen-like ions total energy

In the view point of the Bohr's model, the quantized energy of the hydrogen-like ions is

$$E_n = -\frac{Z^2 \alpha^2 mc^2}{2n^2} \quad (1)$$

where  $\alpha$  denotes the fine structure constant and  $mc^2$  the rest energy of the electron.

On the other hand in the framework of the Bohr's theory, the total energy  $E_n$  and the kinetic energy  $E_c$  satisfy the relation

$$E_n = -E_c.$$

That is to say using Eq. (1)

$$E_n = -\frac{Z^2 \alpha^2 mc^2}{2n^2} = -\frac{1}{2}mv_n^2.$$

This equation shows that, in the view point of the Bohr's semi-classical theory, the electron velocity is quantized and is in the form

$$v_n = \frac{Z\alpha c}{n}. \quad (2)$$

Besides, as well known, the Bohr's model neglects the dependence of the mass electron on the speed and considers also the atomic nucleus as infinitely heavy (this permits to assume it immobile). This model takes not also into account the spin electron discovered 22 years ago (1925) after the Bohr's theory. If the effects of the spin electron on the energy-level of the hydrogen-like ions couldn't be taken into account during the elaboration of the Bohr's theory in 1913 (remembering that the spin were not discovered at this date), at least two corrections to the semi-classical formula given by Eq. (1) may be made. These two corrections are connected to experimental observations and concern

- i) Isotopic shift of the spectral lines due to the dependence of energies on the mass nucleus [2].
- ii) Shift of the relativistic energy-levels of the hydrogen isoelectronic series with respect to the Bohr's semi-classical energy-levels due to the dependence of the mass electron on velocity [1].

For the first correction, the mass nucleus is certainly much bigger than that of the electron, but not infinite. Thus, both electron and nucleus revolve about their common center of gravity which is not exactly identical with the center of the atom. As far as the second correction is concerned, it may be consist of taking into consideration the dependence of the mass electron upon the velocity in the early day of the Bohr's theory (as the Einstein's relativity theory has been performed since 1905). The following study is in this direction turning into account the fact that the hydrogen atom is a weak relativistic atomic system.

## 2.2 Dirac's relativistic expression of the hydrogen-like ions total energy

The Bohr's model successfully predicted the total energies for the hydrogen-like ions in the framework of a semi-classical theory. But, one can put into evidence significant failures of the Bohr's model by solving the Schrödinger's equation for the hydrogen atom as this model ignores relativistic effects due to the motion of the electron and to its properties (the spin for example). The theory of Dirac attempts to unify the quantum mechanics and the relativity theory. For the hydrogen like- ions, the Hamiltonian operator is in the form

$$H = H_0 + W,$$

where  $H_0$  represents the Hamiltonian of the atomic system in a the Coulomb field with the potential  $U(R) = -Ze^2/R$  and  $W$  denotes all the effects neglected in the Bohr's theory.

In the viewpoint of the Dirac's theory,  $W$  can be expanded as follows [1]

$$W = mc^2 - \frac{\mathbf{P}^4}{8m^3c^2} + \frac{1}{2m^2c^2} \frac{1}{R} \frac{dV(R)}{dR} \mathbf{L} \cdot \mathbf{S} + \frac{\hbar^2}{8m^2c^2} \nabla^2 V(R) + \dots$$

Using this development, one can give a correct interpretation of some of the relativistic effects in the hydrogen-like ions

- 1) the dependence of the mass electron on the speed

$$W_{mv} = -\frac{\mathbf{p}^4}{8m^3c^2};$$

- 2) the spin-orbit interaction

$$W_{SO} = \frac{1}{2m^2c^2} \frac{1}{R} \frac{dV(R)}{dR} \mathbf{L} \cdot \mathbf{S};$$

- 3) the fact that the nucleus is not a punctual charge (the Darwin term)

$$W_D = \frac{\hbar^2}{8m^2c^2} \nabla^2 V(R).$$

Then, the fine structure Hamiltonian  $W$  can be written as follows

$$W = W_{mv} + W_{SO} + W_D + \dots.$$

In this development, the electronic spin- nuclear spin interaction is not taken into account.

The effects of the different terms of  $W$  are the following

- 1)  $W_{mv}$  and  $W_D$  permit to put into evidence the global shift of the hydrogen-like ions energy levels;
- 2)  $W_{SO}$  permits to lift up the degeneracy of all the energetical levels characterized by the same value of the orbital quantum number  $\ell$  but with a different value of the inner quantum number  $j = \ell \pm s$ ,  $s$  the spin of the electron.

By solving exactly the Dirac relativistic wave equation, we get [3]

$$E_{nj} = mc^2 \left[ 1 + \left( \frac{Z\alpha}{n - (j + \frac{1}{2}) + \sqrt{(j + \frac{1}{2})^2 - (Z\alpha)^2}} \right)^2 \right]. \quad (3)$$

Expanding this equation in powers of  $Z\alpha$ , we find

$$E_{nj} = mc^2 \left\{ 1 - \frac{1}{2} \frac{(Z\alpha)^2}{n^2} \left[ 1 + \frac{1}{2} \frac{(Z\alpha)^2}{n} \left( \frac{1}{j + \frac{1}{2}} - \frac{3}{4n} \right) \right] + \dots \right\}. \quad (4)$$

The first term on the right hand side of Eq. (4) represents the rest energy of the electron, the second term corresponds to the hydrogen-like ions total energy as given in the Bohr's theory and the last term gives the relativistic correction due to the fine structure Hamiltonian

to order  $(Z\alpha)^4$ . Besides, even the exact solution of Dirac given by Eq. (3) is not a complete description of the hydrogen isoelectronic series (for example it takes not into account the hyperfine coupling due to the electronic spin-nuclear spin interaction, the Lamb shift phenomenon due the quantum properties of the electromagnetic field, ect.), the Dirac's theory permits to put into evidence a lot of phenomena like the spin electron and the fine structure of the hydrogen-like ions, ect. In this paper, we suggest a simple semi-relativistic theory applicable to the hydrogen-like ions and to the helium isoelectronic series where the spin of the electron is ignored. This will permit to put into evidence the global shift of the hydrogen-like ions energy levels without having to invoke the Darwin term  $W_D$  or the Dirac's relativistic theory. In addition, the extension of the present theory to the helium like-ions, permit also to put into evidence a kind of valley of stability in the ground state of two electron systems.

### 2.3 Semi-relativistic total energy of the hydrogen-like ions

In the viewpoint of the Einstein's relativity theory, the momenta  $p$  and the kinetic energy  $E_c$  of a particle of rest mass  $m$  with the speed  $v$  are given by the well knowing formulas [4]

$$p = \frac{mv}{\sqrt{1 - \frac{v^2}{c^2}}}, \quad (5)$$

$$E_c = mc^2 \left( \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} - 1 \right). \quad (6)$$

Introducing the  $\beta$ -parameter defined by  $\beta = v/c$ , Eq. (5) gives for the relativistic ( $p^{\text{rel}}$ ) and classical ( $p^{\text{cl}}$ ) momenta

$$p^{\text{rel}} = \frac{mc\beta}{\sqrt{1 - \beta^2}}, \quad (7)$$

$$p^{\text{cl}} = mc\beta. \quad (8)$$

In Fig. 1, we show the plots  $p = f(\beta)$  in mc units. One can see then, when  $\beta < 0.4$ , the relativistic and classical curves overlap each other. Then, in this area, we can write  $p^{\text{rel}} \approx p^{\text{cl}}$ . This involves the equality between the relativistic and classical kinetic energy. So  $E_c^{\text{rel}} \approx E_c^{\text{cl}}$ . On the other hand, taking into account the fact that, for the hydrogen-like ions, the total energy and the kinetic energy are linked by the relation  $E = -E_c$ , we can put then  $E = -E_c^{\text{cl}} \approx -E_c^{\text{rel}}$ . So, using Eq. (6), we get

$$E = mc^2 \left( 1 - \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} \right). \quad (9)$$

As in the viewpoint of the Bohr's semi-classical theory, the electron velocity is quantized [see Eq. (3)], the semi-relativistic energy (9) is then quantized, so

$$E_n = mc^2 \left( 1 - \frac{1}{\sqrt{1 - \frac{v_n^2}{c^2}}} \right).$$

Using Eq. (3), we obtain finely for H-like ions

$$E_n = mc^2 \left( 1 - \frac{1}{\sqrt{1 - \frac{Z^2 \alpha^2}{n^2}}} \right). \quad (10)$$

In this expression,

- $mc^2$  denotes the rest energy of the electron;
- $\alpha$  is the fine structure constant;
- $Z$  and  $n$  are respectively the charge number and the principal quantum number.

For chronological aspect, it should be underlined that Eq. (10) has been established in 1993, exactly 80 years ago after the establishment of the Bohr's semi-classical formula (1913) given by Eq. (1).

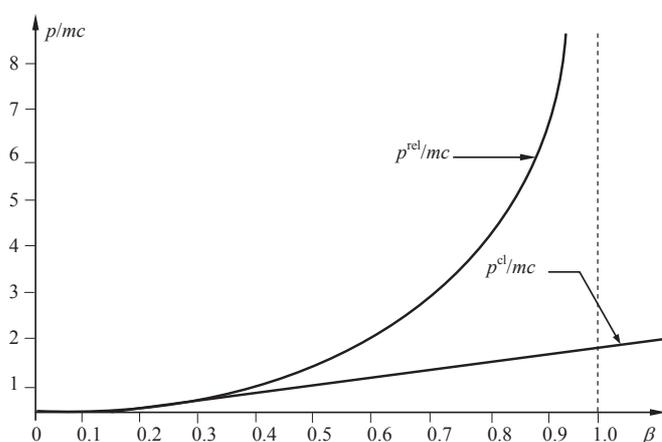


Figure 1: Plots  $p = f(\beta)$  in term of the parameter  $\beta = v/c$ . When  $\beta < 0.4$  the relativistic ( $p^{\text{rel}}$ ) and the classical ( $p^{\text{cl}}$ ) plots overlap. The values of  $p$  are reported in  $mc$  units. In this area, relativistic and classical effects can be considered as in the same order.

## 2.4 Valley of stability in He-like ions

In this section, we extend the present semi-relativistic theory to the helium like-ions using the Screening Constant by Unit Nuclear Charge (SCUNC) method [10–14] which is one of the existing semi-empirical techniques of calculations [15–18]. In the framework of the SCUNC-method, total energy of  $(N\ell, n\ell')^{2S+1}L^\pi$  state is given by

$$E(N\ell n\ell';^{2S+1}L^\pi) = -Z^2 \left( \frac{1}{N^2} + \frac{1}{n^2} [1 - \beta(N\ell n\ell'; Z)]^2 \right) \quad (\text{in Ryd}). \quad (11)$$

In this equation, the principal quantum numbers  $N$  and  $n$  are respectively for the inner and the outer electron of the helium-isoelectronic series. The  $\beta$ -parameters are screening constant by unit nuclear charge expanded in inverse powers of  $Z$  as follows

$$\beta(N\ell n\ell';^{2S+1}L^\pi; Z) = \sum_{k=1}^p f_k \left( \frac{1}{Z} \right)^k, \quad (12)$$

where  $f_k = f_k(N\ell n\ell';^{2S+1}L^\pi)$  are screening constants to be evaluated.

For the ground state which interests our study, Eq. (11) is in the form

$$E(1s^2;^1S^e) = -Z^2 \left( 1 + [1 - \beta(1s^2;^1S^e; Z)]^2 \right) \quad (\text{in Ryd}). \quad (13)$$

As far as the  $\beta$ -parameter is concerned, it is given by (for  $k=1$ )

$$\beta(1s^2;^1S^e; Z) = \frac{f_1}{Z}.$$

Let's us do the change  $f_1 = \sigma$ . We obtain

$$\beta(1s^2;^1S^e; Z) = \frac{\sigma}{Z}.$$

Taking into account this expression, the total energy given by Eq. (13) is written in the form

$$E(1s^2;^1S^e) = -Z^2 \left( 1 + \left[ 1 - \frac{\sigma}{Z} \right]^2 \right) \quad (\text{in Ryd}). \quad (14)$$

Since  $1\text{Ryd} = \alpha^2 mc^2 / 2$ , Eq. (14) can be rewritten in the form

$$E(1s^2;^1S^e) = -\frac{Z^2 \alpha^2 mc^2}{2} \left( 1 + \left[ 1 - \frac{\sigma}{Z} \right]^2 \right). \quad (15)$$

This expression is then a classical one, we can then write

$$E^{\text{cl}}(1s^2;^1S^e) = -\frac{Z^2 \alpha^2 mc^2}{2} \left( 1 + \left[ 1 - \frac{\sigma^{\text{cl}}}{Z} \right]^2 \right). \quad (16)$$

As far as the semi-relativistic expression is concerned, we obtain using Eq. (10)

$$E^{\text{rel}}(1s^2;^1S^e) = mc^2 \left( 1 - \frac{1}{\sqrt{1 - Z^2 \alpha^2}} \right) \left( 1 + \left[ 1 - \frac{\sigma^{\text{rel}}}{Z} \right]^2 \right). \quad (17)$$

Neglecting the relativistic effects due to the dependence of the mass electron upon the speed, Eq. (17) leads to the classical Eq. (16).

### 3 Results and discussion

#### 3.1 Effect of the dependence of the mass electron on the speed on the energy levels of the hydrogen-like ions.

To put into evidence the effects of the dependence of the mass electron upon the speed on the energy levels of the hydrogen-like ions, let's us consider the energetical diagrams as shown in Fig. 2. In this diagram,  $E_n^{\text{srel}}$  and  $E_n^{\text{scl}}$  represent the total energy of the hydrogen atom given respectively by our semi-relativistic formula (1) and by the semi-classical formula of Bohr (1) where one must put  $Z = 1$ . Here we have considered a few levels for  $n = 1-3$ . The energy values are obtained in the basis of [5]: velocity of light  $c = 299792.9 \text{ km sec}^{-1}$ ; electron rest mass:  $m = 9.1085 \times 10^{-28} \text{ g}$ ; fine structure constant:  $\alpha = 1/137.04$ ;  $1 \text{ eV} = 1.60207 \times 10^{-19} \text{ J}$ . Taking into account these values, we obtained:  $mc^2 = 0.51098 \text{ MeV}$ ;  $\alpha^2 = 5.3248 \times 10^{-5}$ . Fig. 2 indicates clearly that, due to the dependence of the mass electron on the speed, the relativistic energy levels are shifted down with respect to the semi-classical energy

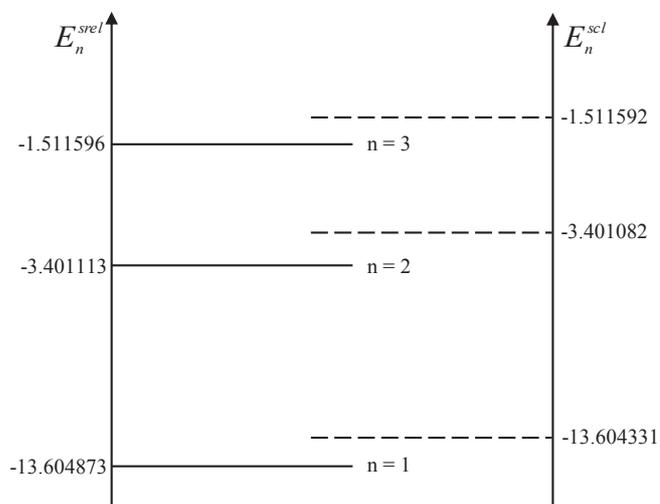


Figure 2: Effect of the dependency of the mass of electron with velocity on the total energetical levels of the hydrogen atom. The relativistic levels are shifted down with respect to the non perturbed levels in good agreement with experiment. Energy units are expressed in eV.

levels in good agreement with experiment [1]. But, one can see that, when the principal quantum number increases, the distance between the relativistic and the semi-classical levels decreases. For example, in the particular case of  $n=3$  level, the energetical difference  $E^{\text{scl}} - E^{\text{srel}} = -1.511592 + 1.511596 = 0.000004$ . This points out that, the hydrogen atom is a very weak relativistic system and in high excited states, it can be considered as a classical atomic system.

### 3.2 Limit of validity of the present semi-relativistic expression

Our formula (10) is valid in the area  $0 \leq \beta < 0.4$ . As  $\beta = v/c$ , Eq. (10) can be used for all the hydrogen-like ions with the condition

$$0 \leq v_n/c < 0.4.$$

By use of Eq. (3), this condition becomes

$$Z\alpha/n < 0.4. \quad (18)$$

- For the ground state  $n=1$ , we get from Eq. (18)  $Z = 0.4/\alpha$ . That means using the value of the fine structure constant  $\alpha = 1/137.04$

$$Z < 54.816. \quad (19)$$

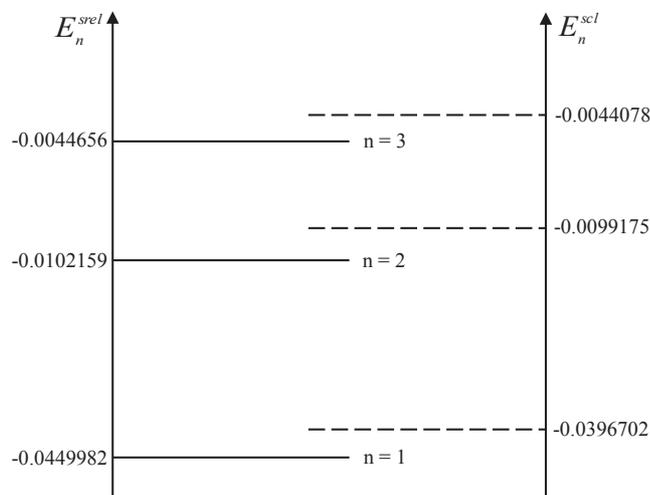


Figure 3: Effect of the dependency of the mass of electron with velocity on the total energy levels of the  $\text{Xe}^{53+}$  hydrogen-like ion. The relativistic levels are shifted down with respect to the non perturbed levels in good agreement with experiment. Energy units are expressed in MeV.

As for the xenon atom  $Z = 54$ , this result indicates that, in the ground state, all the hydrogen-like ions from H to  $\text{Xe}^{53+}$  can be considered as weak relativistic atomic system. Then, the effects of the dependence of the mass electron upon the speed on the energy levels of these atomic systems can be put into evidence by use of Eq. (10). In Fig. 3, we have indicated the shift of the relativistic energy levels with respect to the semi-classical energy levels for the  $\text{Xe}^{53+}$  ion. For excited states  $n > 1$ , we get again from Eq. (18)  $Z < 0.4n/a$ . For the lowest state  $n = 2$ , we find using  $a = 1/137.04$

$$Z < 109.632. \quad (20)$$

This result shows that, in the excited states, all the natural hydrogen-like ions can be considered as weak relativistic atomic systems. Then, our formula (10) could be applied for such systems.

### 3.3 Calculations of the energetical shifts

#### 3.3.1 According to the Dirac's theory

Developing the Dirac's truncated solution (4), we obtain after arrangement

$$E_{nj} = -\frac{Z^2\alpha^2 mc^2}{2n^2} - \frac{Z^4\alpha^4 mc^2}{2n^3} \left( \frac{1}{j+\frac{1}{2}} - \frac{3}{4n} \right). \quad (21)$$

The Hamiltonian of the hydrogen-like ions can be written in the form

$$H = H_0 + W_j^{mv}. \quad (22)$$

In this expression,  $W_j^{mv}$  denotes the eigenvalue of the fine structure Hamiltonian  $W_j^{mv}$ . Then we can state

$$\langle W_{n,j}^{mv} \rangle = -\frac{Z^4\alpha^4 mc^2}{2n^3} \left( \frac{1}{j+\frac{1}{2}} - \frac{3}{4n} \right). \quad (23)$$

By use of this equation, we find respectively for the levels  $1s_{1/2}$ ,  $2s_{1/2}$ ,  $2p_{1/2}$ ,  $2p_{3/2}$ ,  $3s_{1/2}$ ,  $3p_{1/2}$ ,  $3p_{3/2}$ ,  $3d_{3/2}$  and  $3d_{5/2}$ , the following results

- For  $1s_{1/2}$  level,

$$\langle W_{1,\frac{1}{2}}^{mv} \rangle = -\frac{1}{8} Z^4 \alpha^4 mc^2. \quad (24a)$$

- For  $2s_{1/2}$  and  $2p_{1/2}$  levels,

$$\langle W_{2,\frac{1}{2}}^{mv} \rangle = -\frac{5}{128} Z^4 \alpha^4 mc^2. \quad (24b)$$

- For  $2p_{3/2}$  level,

$$\langle W_{2,\frac{3}{2}}^{mv} \rangle = -\frac{1}{128} Z^4 \alpha^4 mc^2. \quad (24c)$$

- For  $3s_{1/2}$  and  $3p_{1/2}$  levels,

$$\langle W_{3, \frac{1}{2}}^{mv} \rangle = -\frac{1}{72} Z^4 \alpha^4 mc^2. \quad (24d)$$

- For  $3p_{3/2}$  and  $3d_{3/2}$  levels,

$$\langle W_{3, \frac{3}{2}}^{mv} \rangle = -\frac{1}{216} Z^4 \alpha^4 mc^2. \quad (24e)$$

- For  $3d_{5/2}$  level,

$$\langle W_{3, \frac{5}{2}}^{mv} \rangle = -\frac{1}{648} Z^4 \alpha^4 mc^2. \quad (24f)$$

These results indicate the degeneracy of all the levels with the same value of the  $j$ -inner quantum number but with a different value of the  $\ell$ -orbital quantum number.

### 3.3.2 According to the integral calculation

The three terms of the fine structure Hamiltonian in the viewpoint of the Dirac's theory, can be calculated directly. If  $\Phi(r)$  represents the wave function associated to a stationary state of the hydrogen-like ions, the average value of  $W$  is given by

$$\langle W \rangle = \frac{\langle \Phi | W | \Phi \rangle}{\langle \Phi | \Phi \rangle},$$

with  $\langle W \rangle = \langle W_{mv} \rangle + \langle W_{SO} \rangle + \langle W_D \rangle$ .

These average values are easily calculated for the hydrogen atom [1]. Generalisation of the results obtained in the case of the hydrogen-like ions gives

- For  $1s_{1/2}$ ,

$$\langle W_{mv} \rangle = -\frac{5}{8} Z^4 \alpha^4 mc^2; \quad \langle W_D \rangle = \frac{1}{2} Z^4 \alpha^4 mc^2; \quad \langle W_{SO} \rangle = 0.$$

Then

$$\langle W \rangle 1s_{1/2} = -\frac{1}{8} Z^4 \alpha^4 mc^2. \quad (25a)$$

- For  $2s_{1/2}$  level,

$$\langle W_{mv} \rangle = -\frac{13}{128} Z^4 \alpha^4 mc^2; \quad \langle W_D \rangle = \frac{1}{16} Z^4 \alpha^4 mc^2; \quad \langle W_{SO} \rangle = 0.$$

Then

$$\langle W \rangle 1s_{1/2} = -\frac{5}{8} Z^4 \alpha^4 mc^2. \quad (25b)$$

- For  $2s_{1/2}$  level,

$$\langle W_{mv} \rangle = -\frac{13}{128} Z^4 \alpha^4 mc^2; \quad \langle W_D \rangle = \frac{1}{16} Z^4 \alpha^4 mc^2; \quad \langle W_{SO} \rangle = 0.$$

Then

$$\langle W \rangle_{2s_{1/2}} = -\frac{5}{8} Z^4 \alpha^4 mc^2. \quad (25c)$$

• For  $2p_{1/2}$  level,

$$\langle W_{mv} \rangle = -\frac{7}{384} Z^4 \alpha^4 mc^2; \quad \langle W_D \rangle = 0; \quad \langle W_{SO} \rangle = -\frac{1}{48} Z^4 \alpha^4 mc^2.$$

Then

$$\langle W \rangle_{2p_{1/2}} = -\frac{5}{128} Z^4 \alpha^4 mc^2. \quad (25d)$$

• For  $2p_{3/2}$  level,

$$\langle W_{mv} \rangle = -\frac{7}{384} Z^4 \alpha^4 mc^2; \quad \langle W_D \rangle = 0; \quad \langle W_{SO} \rangle = \frac{1}{96} Z^4 \alpha^4 mc^2.$$

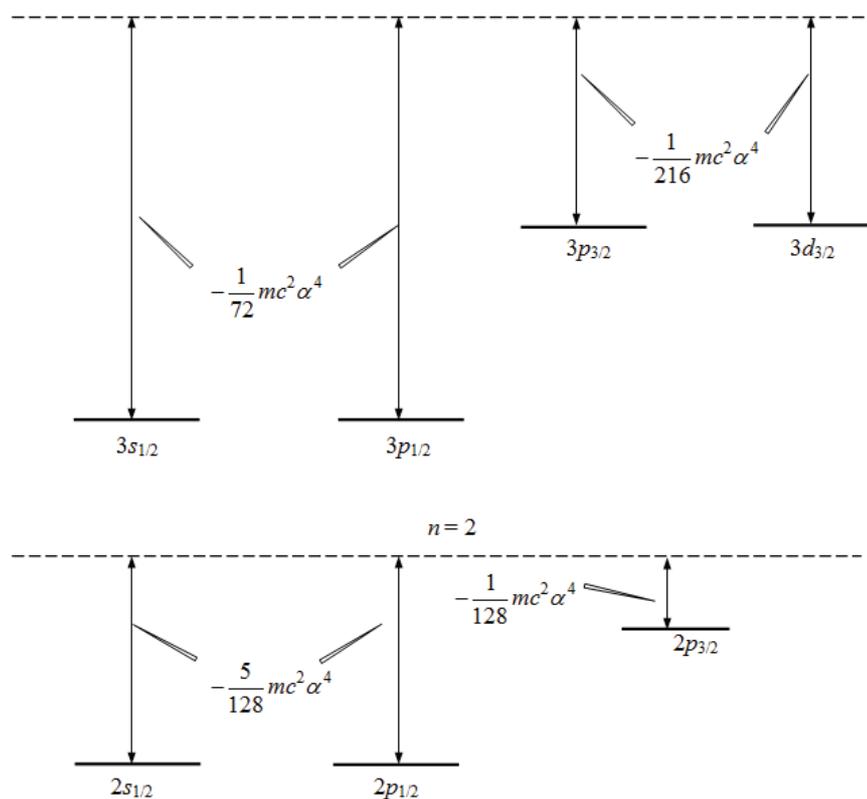


Figure 4: Fine structure of the  $n=2-3$  levels of the hydrogen atom. Due to the effect of the fine structure Hamiltonian  $W$ , the  $n=2-3$  levels are split up into three fine structure levels: three confounded levels ( $2s_{1/2}$ ,  $2p_{1/2}$ ), ( $3s_{1/2}$ ,  $3p_{1/2}$ ) and ( $3p_{3/2}$ ,  $3d_{3/2}$ ) and two simple levels  $3p_{3/2}$  and  $3d_{5/2}$ . The energetical shifts are the same for ( $2s_{1/2}$ ,  $2p_{1/2}$ ), ( $3s_{1/2}$ ,  $3p_{1/2}$ ) and ( $3p_{3/2}$ ,  $3d_{3/2}$ ) levels.

Then

$$\langle W \rangle_{2p_{3/2}} = -\frac{1}{128} Z^4 \alpha^4 mc^2. \quad (25e)$$

The above results give the positions of the  $2s_{1/2}$ ,  $2p_{1/2}$  and  $2p_{3/2}$  levels with respect to the non-perturbed energy of the  $n=2-3$  levels for the hydrogen atom as shown in Fig. 4. Due to the effects of the  $W$ -fine structure Hamiltonian, the  $n=2-3$  levels are split up into three fine structure levels: three confounded levels ( $2s_{1/2}$ ,  $2p_{1/2}$ ), ( $3s_{1/2}$ ,  $3p_{1/2}$ ) and ( $3p_{3/2}$ ,  $3d_{3/2}$ ) and two individual levels  $3p_{3/2}$  and  $3d_{5/2}$ . In the particular case of  $2s_{1/2}$  and  $2p_{1/2}$  levels, the radio spectroscopy experiments of Lamb and Retherford in 1947 as described in Ref. [2], have shown that these two levels are separated as indicated in Fig. 5. For the hydrogen atom, the difference frequency is equal to  $1057.845 \pm 0.09$  Hz. This difference (and generally all difference between the fine structure levels with the same value of the principal quantum number  $n$  and the inner quantum number  $j$  but with a different value of the orbital quantum number  $\ell$ ) is called the Lamb shift. On the theoretical sides, the quantum electrodynamics theory gives this difference at  $1057.864 \pm 0.014$  Hz [2], which is in very good agreement with the radio spectroscopy experiments of Lamb and Retherford.

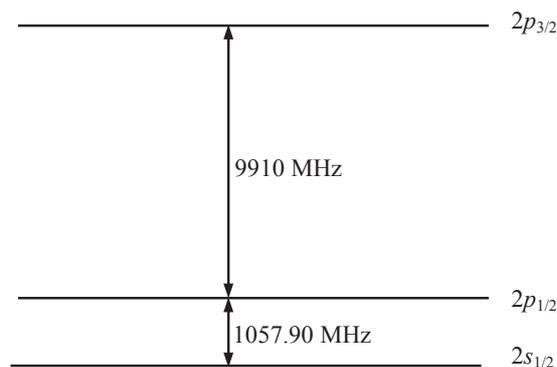


Figure 5: Three fine structure levels labelled  $2s_{1/2}$ ,  $2p_{1/2}$ ,  $2p_{3/2}$ . Taking into account the quantum properties of the electromagnetic field, the degeneracy of the  $2s_{1/2}$  and  $2p_{1/2}$  is elevated (this corresponds to the Lamb shift phenomenon). Here, we indicate the difference frequency between  $2s_{1/2}$  and  $2p_{1/2}$  equals to  $1057.845 \pm 0.09$  Hz according to the radiospectroscopy experiments of Lamb and Retherford for the hydrogen atom.

### 3.3.3 According to the present semi-relativistic theory

Let's us expand our semi-relativistic formula (10) in powers of  $Z\alpha$ . We obtain

$$E_n = mc^2 \left[ 1 - \left( 1 + \frac{Z^2 \alpha^2}{2n^2} + \frac{3}{8} \frac{Z^4 \alpha^4}{n^4} + \dots + \theta \left( \frac{Z\alpha}{n} \right)^n \right) \right]. \quad (26)$$

To 2-order approximation, Eq. (26) yields

$$E_n = -\frac{Z^2 \alpha^2 mc^2}{2n^2} - \frac{3}{8} \frac{Z^4 \alpha^4 mc^2}{n^4} - \dots. \quad (27)$$

According to Eq. (22), we can write again

$$H = H_0 + W_{mv}. \quad (28)$$

Comparing Eqs. (27) and (28), one can see that, the second term in the right hand side of Eq. (27) corresponds to the eigenvalue of the fine structure Hamiltonian  $W_{mv}$ . Then we can get

$$\langle W_n^{mv} \rangle = -\frac{3}{8} \frac{Z^4 \alpha^4 m c^2}{n^4}. \quad (29)$$

Let's us now move on invoking the equipartition theorem that constitutes an important result in thermodynamics, statistical mechanics and kinetic theory [6,7]. As developed above, the present theory is based on the condition that the relativistic and classical kinetic energies satisfy the relation  $E = -E_c^{\text{cl}} \approx -E_c^{\text{rel}}$ , where  $E$  represents the total energy of the hydrogen-like ions. As the spin electron is ignored, the motion of the electron corresponds to 3 degrees of freedom (as defined by the three coordinates of the speed  $v_x, v_y, v_z$ ). Then according to the equipartition theorem, the average kinetic energy is divided up equally between all the degrees of freedom. So, on the side of the present semi-relativistic theory, to each  $x$ -degree of freedom, corresponds the average energetical shift

$$\langle W_{mv} \rangle_n = \frac{1}{3} \langle W_n^{mv} \rangle.$$

From Eq. (29), we get finally

$$\langle W_{mv} \rangle_n = -\frac{1}{8} \frac{Z^4 \alpha^4 m c^2}{n^4}. \quad (30)$$

Then, due to the dependence of the mass electron on speed, the  $n$ -levels of the hydrogen-like ions are shifted down with the quantities

- For  $n=1$ ,

$$\langle W_{mv} \rangle_1 = -\frac{1}{8} Z^4 \alpha^4 m c^2. \quad (31a)$$

- For  $n=2$ ,

$$\langle W_{mv} \rangle_2 = -\frac{1}{128} Z^4 \alpha^4 m c^2. \quad (31b)$$

- For  $n=3$ ,

$$\langle W_{mv} \rangle_3 = -\frac{1}{648} Z^4 \alpha^4 m c^2. \quad (31c)$$

### 3.4 Comparison with the theoretical calculations

If we consider the results given by Eqs. (24) and (25), one can remark that

$$\langle W_{mv} \rangle^{PC} = \langle W \rangle^{IC} 1s_{\frac{1}{2}} = \left\langle W_{1, \frac{1}{2}}^{mv} \right\rangle^{DC} = -\frac{1}{8} Z^4 \alpha^4 mc^2, \quad (32a)$$

$$\langle W_{mv} \rangle_2^{PC} = \langle W \rangle^{IC} 2p_{\frac{3}{2}} = \left\langle W_{2, \frac{3}{2}}^{mv} \right\rangle^{DC} = -\frac{1}{128} Z^4 \alpha^4 mc^2, \quad (32b)$$

$$\langle W_{mv} \rangle_3^{PC} = \left\langle W_{3, \frac{5}{2}}^{mv} \right\rangle^{DC} = -\frac{1}{648} Z^4 \alpha^4 mc^2. \quad (32c)$$

In Eq. (32), the subscripts signification are the following: PC represents the Present Calculations, IC represents the Integral Calculations, and DC represents the Dirac's Calculations.

These results point out that, our semi-relativistic shift (30) in connection with the equipartition theorem coincides with the non degenerated energy levels of the spectroscopic terms  $1s_{1/2}$ ,  $2p_{3/2}$  and  $3d_{5/2}$ . Henceforth, we can generalize this result. For a non degenerated level corresponding to the maximum value of the inner quantum number  $j = \ell \pm s$ , the energetical shift due to the fine structure Hamiltonian  $W$  is given by the formula from Eq. (30)

$$\langle W_{mv} \rangle_{j=n-\frac{1}{2}} = -\frac{1}{8} \frac{Z^4 \alpha^4 mc^2}{n^4}. \quad (33)$$

In the particular case of the  $n=4$  level, Eq. (33) gives for to the  $4f_{7/2}$  term

$$\langle W_{mv} \rangle_{\frac{7}{2}} = \frac{1}{2048} Z^4 \alpha^4 mc^2. \quad (34)$$

Using Eq. (33) obtained from the Dirac's relativistic theory, we find

$$\left\langle W_{4, \frac{7}{2}}^{mv} \right\rangle = \frac{Z^4 \alpha^4 mc^2}{2 \times 4^3} \left( \frac{1}{\frac{7}{2} + \frac{1}{2}} - \frac{3}{4 \times 4} \right) = -\frac{Z^4 \alpha^4 mc^2}{2048}.$$

We get then the same result (34). This agreement indicates the exactitude of Eq. (33). Subsequently, Eq. (33) permits to calculate directly the energetical shift of any non-degenerated level of the hydrogen-like ions without needing to invoke the Dirac's theory or the integral calculations. On the other hand, it is interesting to underline that, our semi-relativistic formula (10) contains the semi-classical theory of Bohr (1). In the same way, the Dirac's relativistic formula (3) contains that of the present work. This is clearly indicated below. If we consider Eq. (1) and the expansions (4) and (27), we get after arrangement

$$E_n = -\frac{Z^2 \alpha^2 mc^2}{2n^2} \quad (\text{Bohr's semi-classical results})$$

$$E_n = -\frac{Z^2 \alpha^2 mc^2}{2n^2} - \frac{3 Z^4 \alpha^4 mc^2}{8 n^4} \quad (\text{Present semi-relativistic results})$$

$$E_n = -\frac{Z^2 \alpha^2 mc^2}{2n^2} - \left[ -\frac{3 Z^4 \alpha^4 mc^2}{8 n^4} + \frac{1}{2} \frac{Z^4 \alpha^4 mc^2}{n^3 \left( j + \frac{1}{2} \right)} \right] \quad (\text{Dirac's relativistic results})$$

### 3.5 Valley of stability in the helium-like ions

Let's us evaluate empirically the values of the classical and relativistic screening constants using Eqs. (16) and (17). In this purpose, we use the experimental total energies [8, 9] of some helium-like ions ( $Z = 2-10$ ). From Eqs. (16) and (17), we obtain the results quoted in Table 1. In order to enlighten the differences between the values of the classical ( $\sigma^{\text{cl}}$ ) and the relativistic ( $\sigma^{\text{rel}}$ ) screening constants, let's us draw the plot  $\sigma = f(Z)$  in terms of the nuclear charge  $Z$  of the helium-like ions. The results obtained are shown in Figs. 6 and 7. From these figures, it is seen that the classical screening constant  $\sigma^{\text{cl}}$  decreases monotony when increasing the nuclear charge. As far as the relativistic screening constant is concerned, Fig. 7 indicates clearly that the  $\sigma^{\text{rel}}$  screening constant decreases up to  $Z = 5$  ( $\text{B}^{3+}$ ) and after, increases when increasing the nuclear charge. The plot is like a valley where the bottom is occupied by the  $\text{B}^{3+}$ -helium like ion. It is well know that atoms can be ionized by bombardment using radiation sources. But, the more usual process of ionization is the transfer of electrons between atoms with respect to their electronegativity properties. Such a transfer is generally driven by the reach of stable "closed shell" electronic configurations (for most of the atoms, the stable shell contains eight electrons). As a result, the oxygen atom for instance, gains two electrons during the natural ionization process. So the natural ion obtain is  $\text{O}^{2-}$ . Then, Li, Be and B which are electropositive atoms, can only have positive electric charge after the natural ionization process and become respectively  $\text{Li}^+$ ,  $\text{Be}^{2+}$  and  $\text{B}^{3+}$ . But, all the non metallic atom, like C, N, O, F, Cl, ect., cannot lose electrons during a natural ionization process as they are not electropositive atomic systems. This is shown by the relativistic behavior of the screening constant as indicated in Fig. 7. In summary, only the closed shell core of  $\text{Li}^+$ ,  $\text{Be}^{2+}$  and  $\text{B}^{3+}$  are stable and that of  $\text{C}^{4+}$ ,  $\text{N}^{5+}$ ,  $\text{O}^{6+}$ ,  $\text{F}^{7+}$ ,  $\text{Cl}^{8+}$ , ect, are instable and these ions can only exist in

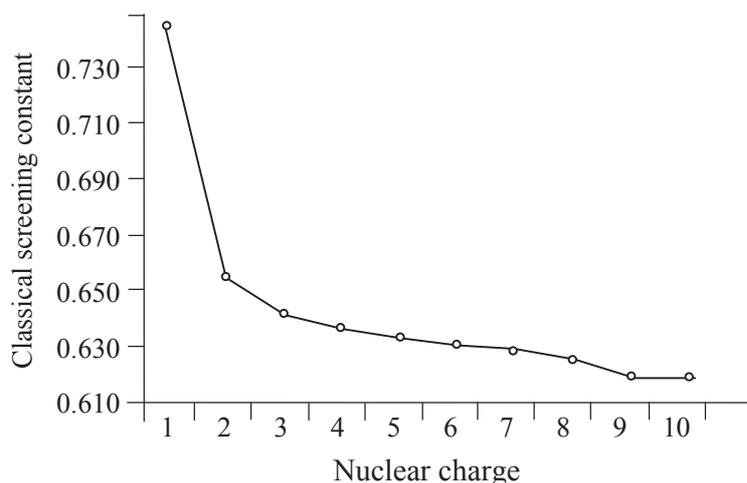


Figure 6: Classical plot  $\sigma^{\text{cl}} = f(Z)$  in terms of the nuclear charge  $Z$  of the helium-like ions. The classical screening constant  $\sigma^{\text{cl}}$  decreases monotony when increasing the nuclear charge.

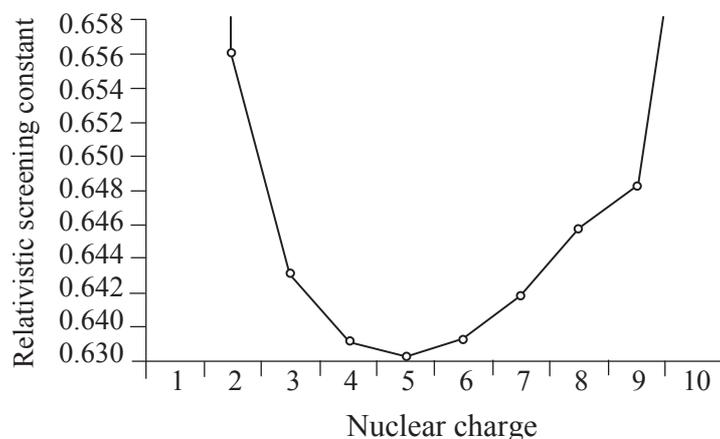


Figure 7: Relativistic plot  $\sigma^{\text{rel}}=f(Z)$  in terms of the nuclear charge  $Z$  of the helium-like ions. The relativistic screening constant  $\sigma^{\text{rel}}$  decreases up to  $Z=5$  ( $\text{B}^{3+}$ ) and after, increases when increasing the nuclear charge. The plot is like a valley where the bottom is occupied by the  $\text{B}^{3+}$ -helium like ion.

Table 1: Comparison between the classical ( $\sigma^{\text{cl}}$ ) and relativistic ( $\sigma^{\text{rel}}$ ) screening constant for some helium-like ions ( $Z=2-10$ ). We have indicated in the second column of the table, the experimental energy of the ground state of each considered helium-like ions (in eV).

Helium-like ions	Ground state energy (in eV)	Classical screening constant ( $\sigma^{\text{cl}}$ )	Relativistic screening constant ( $\sigma^{\text{rel}}$ )
He	79.01 <sup>a</sup>	0.655 7	0.656 0
Li <sup>+</sup>	198.09 <sup>b</sup>	0.642 2	0.643 2
Be <sup>2+</sup>	371.60 <sup>b</sup>	0.636 6	0.639 2
B <sup>3+</sup>	599.58 <sup>b</sup>	0.633 3	0.638 2
C <sup>4+</sup>	882.05 <sup>b</sup>	0.630 7	0.639 2
N <sup>5+</sup>	1219.07 <sup>b</sup>	0.628 2	0.641 8
O <sup>6+</sup>	1610.69 <sup>b</sup>	0.625 5	0.645 8
F <sup>7+</sup>	2057.68 <sup>b</sup>	0.619 3	0.648 3
Ne <sup>8+</sup>	2557.94 <sup>b</sup>	0.618 9	0.705 9

<sup>a</sup> Ref. [8].

<sup>b</sup> Ref. [9].

hot laboratory or astrophysical plasmas. It is this important result that one can retain through the behavior of the relativistic screening constant whose plot is like a valley of stability.

## 4 Conclusion

In this paper, we have presented a simple semi-relativistic theory for the hydrogen-like ions that could be considered as a first correction of the Bohr's semi-classical theory. The possibility to interpret physically the relativistic effect due to the variation of the mass electron with

velocity on the energy levels of the hydrogen isoelectronic series without invoking the Dirac's theory is demonstrated in this work. In addition, it is shown that, for the ground state of two electron systems, the relativistic screening constant  $\sigma^{\text{rel}}$  decreases when increasing the nuclear charge up to  $Z = 5$ . Beyond,  $\sigma^{\text{rel}}$  increases when increasing  $Z$  and, the plot  $\sigma^{\text{rel}} = f(Z)$  is like a valley of stability where the bottom is occupied by the  $B^{3+}$ -helium-like ion. As a result, only He,  $Li^+$ ,  $Be^{2+}$  and  $B^{3+}$  exist in the natural matter in low temperature. All the other helium-like positive-ions, such as  $C^{4+}$ ,  $N^{5+}$ ,  $O^{6+}$ ,  $F^{7+}$ ,  $Ne^{8+}$ , ..., can only exist in hot laboratory and astrophysical plasmas.

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