Electron Deep Orbits of the Hydrogen Atom

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Abstract. This work continues our previous work [1] and in a more developed form [2]), on electron deep orbits of the hydrogen atom. An introduction shows the importance of the deep orbits of hydrogen (H or D) for research in the LENR domain, and gives some general considerations on the EDO (Electron Deep Orbits) and on other works about deep orbits.
A first part recalls the known criticism against the EDO and how we face it. At this occasion we highlight the difference of resolution of these problems between the relativistic Schrödinger equation and the Dirac equation, which leads for this latter, to consider a modified Coulomb potential with finite value inside the nucleus.
In the second part, we consider the specific work of Maly and Va'vra [3], [4]) on deep orbits as solutions of the Dirac equation, so-called Deep Dirac Levels (DDLs). As a result of some criticism about the matching conditions at the boundary, we verified their computation, but by using a more complete ansatz for the "inside" solution. We can confirm the approximate size of the mean radii $<r>$ of DDL orbits and that $<r>$ decreases when the Dirac angular quantum number k increases. This latter finding is a self-consistent result since (as distinct from the atomic-electron orbitals) the binding energy of the DDL electron increases (in absolute value) with k. We observe that the essential element for obtaining deep orbits solutions is special relativity.

Keywords: Deep electron levels, LENR, Relativistic quantum Physics, Singular solutions

Introduction

For many decades, the question of the existence of electron deep levels or electron deep orbits (EDOs) for the hydrogen atom led to numerous works and debates. Why once more a study on this subject? For several reasons:

- EDOs are predicted by relativistic quantum equations, with mean radius of the orbitals of order femto-meter.
- So, hydrogen atoms (including deuterium) with electron deep orbits (femto-atoms) can facilitate processes of LENR inside condensed matter, the avoidance of nuclear fragmentation in D-D => ^{4}He fusion reactions, and a means of increasing the rate of energy transfer between an excited nucleus and the surrounding lattice
- Moreover, femto-atoms could create femto-molecules and combine with lattice nuclei for transmutation without energetic radiations.
- By accepting the reality of a non-singular central potential within a nuclear region, many mathematical arguments against anomalous solutions of the relativistic equations no longer pertain.
- Numerical methods now allow prediction of properties and features of the EDOs.

The statements above for the importance of deep-electron orbits to LENR are factual. However, they convey neither the true criticality of the concept to cold fusion (CF) theory nor the evidence (and publications) to support these statements. The first part of this introduction will attempt to do both for the statements pertaining to CF. The second part of the introduction will be specific to the theme of the paper 'validating the relativistic models for the deep orbits'.

It was recognized early in the CF development that the best (perhaps the only) means of fusion at low temperatures and energies was to increase the time that negative charge spends between fusing nuclei. This means of overcoming the Coulomb barrier between nuclei is a continuing theme and is addressed in most models of LENR (see for example, "Extensions to physics: what cold fusion teaches," [5]). The other side of the problem was emphasized in 2013 (by Akito Takahashi at ICCF-15): "even if the Coulomb barrier were to be lowered to zero, D+D fusion would still lead to ^{4}He-fragmentation products, not to the observed atomic ^{4}He and heat of CF." This problem is perhaps best addressed by the means and consequences of electron decay to the deep orbits ("Tunneling Beneath the ^{4}He* Fragmentation Energy,"[6] and "From the Naught Orbit to He4 Ground State" [7]).
With the recognition that deep-orbit electrons can explain some of the fundamental problems of cold fusion, a more complete study of the nature and effects of these relativistic electrons was begun ("Deep-electron orbits in Cold Fusion"[8]). An important side issue of this study was the nature of electromagnetic radiation from the deep-orbit electrons and the ability of deep-orbit electrons to transfer energy between an excited nucleus and the lattice ("Deep-Orbit-Electron Radiation Emission in Decay from 4He*# to 4He," [9]). As confidence grew in the CF results for transmutation in both the PdD and

NiH systems, the concept of longer-lived ‘femto-atoms’, their nature and their consequences, became the subject of analysis (“Femto-atoms and Transmutation” [10] and “Femto-Helium and PdD Transmutation” [11]). These studies led to an understanding of 3-body fusion processes (femto-atom + nucleus) to explain both transmutation without hard radiation and selective radio-isotope remediation.

The least-resolved portion of the deep-orbit electron scenario is why the deep levels are not immediately filled from atomic orbitals and why are they not readily observed? If they are not able to be populated in the natural environment, then how are we to populate these levels. This latter question has been addressed in part by (“Lochon Catalyzed D-D Fusion in Deuterated Palladium in the Solid State” [12], “Composite model for LENR in linear defects of a lattice” [13], and “Pictorial description for LENR in linear defects of a lattice,” [14]).

Since the deep-orbit model can explain all of the observed CF results that have been addressed and is based on the fundamental equations of relativistic quantum mechanics, it should be readily accepted. However, it has been rejected for over 50 years (perhaps 75 years) for primarily mathematical reasons. It is hoped that, with the cooperation of a mathematician and a physicist in the present authors, the non-physical reasons for rejecting the concept can be eliminated and a firm mathematical base can be laid that would lead to acceptance of both the deep orbits and a theory for cold fusion.

There are, in the literature, various and numerous theoretical methods to define a state of the hydrogen atom with electron deep orbits (EDO). Some authors use the term *hydrino* for denoting the special deep-orbit hydrogen states owing to the work of Mills [15] on the hypothetical existence of H atoms with orbit levels under the Bohr ground level and where the values of orbit radii are fractional values of the Bohr radius. Here we do not use this term, a physical concept specifically attached to the cited work, because it is not deduced from (standard) relativistic quantum equations.
With the quantum equations habitually used in the literature for computing the bound states of the H atom, we can note that there is in general a crossroad with a choice of value or a choice of sign for a square root in a parameter. According to which path is chosen, the resolution process leads either to the usual “regular” solution or to an unusual one called an "anomalous" solution; this latter is rejected in the Quantum Mechanics Textbooks. Nevertheless, we can note that *every anomalous solution is not necessarily one* with EDO.

Why do we emphasize here the use of *relativistic* quantum equations?
For (at least) two reasons:

- 1. Only the relativistic equations can predict EDOs with mean radius of order femto-meter.

We can even give a simple mathematical reason for this fact.
So, for example, one can see that with a non-relativistic Schrödinger equation, one can obtain “anomalous” solutions, but they are not EDOs.

- 2. With an EDO having a mean radius of order femto-meter, the Coulomb potential energy is so high that the electron is necessarily relativistic [1].

Nevertheless, we can note the works of Vigier [16] and Barut [17], then Samsonenko et al. [18], Dragic et al [19], on possible electron tight orbits under the Bohr level for atom H (or D), and even “tight molecules” with energy of several keV. These are treated in a non-relativistic framework, because the energies are not high enough to justify special relativity. These works take into account magnetic interactions such as spin-orbit and spin-spin (electron-nucleus), which at the scale of classical atomic orbitals, have a very weak impact, but will remove level degeneracies. Nevertheless, at distances closer to nucleus, these magnetic interactions can modify the Coulomb potential into a series of inverse-power potentials of the following form, as indicated also in the work of OzceliK et al. [20]:

$$V(r) = A/r + B/r^2 + C/r^3 + D/r^4 , \qquad (1)$$

Of course $A < 0$ since the first term corresponds to the Coulomb potential, but if $D > 0$ and $C < 0$, one has a “repulsive core” and a possible deep potential well. The methods of solutions are “semi-numerical” approximations and the authors indicate little information about energy values for atom H: we noted the value 40 keV in [18] as a maximum.

The corresponding orbitals are in fact much less deep than the EDO obtained by the relativistic quantum equations. On the other hand, the considered magnetic interactions should be obviously much stronger for EDO and could eliminate the question of the singular point of the Coulomb potential and the problems associated with this singular point.
In figure 1 and figure 2, we represent a potential like in (1) having three zeros, with $B > 0$, $C < 0$, $D > 0$. Of course, the values on the axis have no physical meaning: it is only a simulation.

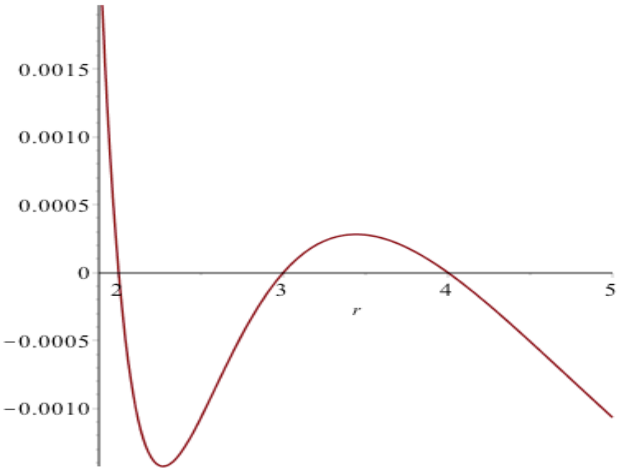

Fig.1. $V(r)$ for $r \le 5$

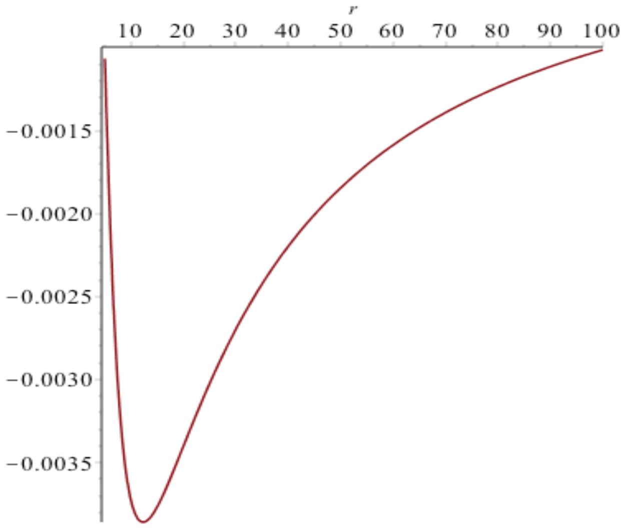

Fig. 2. $V(r)$ for $0 \le r \le 100$

Finally, concerning the magnetic effects on the Coulomb potential, we can note a very subtle effect due to the "Anomalous Magnetic Moment" of the electron. It can be taken into account in the Dirac equation, under the form of an additional term in inverse-power: $-\mu_a \alpha/r^2$. In fact, it does not directly act on the central potential, but it is added to the non-diagonal terms of the 2X2 matrix representing the radial Dirac operator (2). As indicated by Thaller [21] [22], it acts as a repulsive interaction that "forces the wavefunction away from the singularity." So, it also eliminates the problems related to this singularity.

$$D_r = \begin{pmatrix} mc^2 + V(r) & \hbar c\left(-\frac{d}{dr} + \frac{k}{r}\right) - \mu_a \boldsymbol{V'(r)} \\ \hbar c\left(\frac{d}{dr} + \frac{k}{r}\right) - \mu_a \boldsymbol{V'(r)} & -mc^2 + V(r) \end{pmatrix} \tag{2}$$

I. Arguments against the EDO states

The arguments against the EDO states (assuming a singular 1/r Coulomb potential) have been already exposed in detail in [1], as well as the possible solutions to resolve these questions. They concern only the radial solutions of the quantum equations and they are the following ones:

- The wavefunction has a singular point at the origin.
- The wavefunction is not 'square integrable'.
- The 'orthogonality criterion' cannot be satisfied.

We can note all three problems are related to the singularity of the Coulomb potential at $r = 0$.

- We noted also a fourth question: the strength of the binding seems to increase when the coupling strength decreases.

First, we cope with this fourth question, as it is not related to the singularity of the potential.

I-1. The behavior of the binding energy while the coupling strength decreases

One can consider variations of the coupling strength $\gamma = Z\alpha$, where α is the coupling constant, and to examine the consequence of such variations on atomic orbitals. We can cite, for example, the work of Thaller [22], where properties of the Dirac operator are analyzed, in particular for heavy atoms ($Z \gg 1$).
It can also be very instructive to make the following "thought experiment": to imagine variations of the coupling constant α and observe consequences on eigenfunctions of quantum equation. Doing this in

[23], Dombey points to a very strange phenomenon concerning the EDO solutions of the Klein-Gordon equation: when α decreases and tends towards 0, the binding energy of the electron increases in absolute value and tends towards its maximum. He observes the same phenomenon with the 2-D Dirac equation. To simplify, as in the cited paper, we consider only the “anomalous” solutions of the Klein-Gordon equation with angular momentum $l = 0$. The expression of the total energy of the electron is the following:

$$E_N = mc^2[1+\frac{\alpha^2}{[N+\frac{1}{2}-\sqrt{(\frac{1}{4}-\alpha^2)}]^2}]^{-1/2} \tag{3}$$

The deep orbits are obtained only if the radial quantum number $N = 0$. We recall further the general conditions for deep orbits. With $N = 0$, the sub-expression $\Delta = N + \frac{1}{2} - (\frac{1}{4} - \alpha^2)^{1/2}$ can be reduced to α^2 and then $E_0 \sim mc^2\alpha$. So, if $\alpha \to 0$, we have the total energy $E_0 \to 0$, and this implies that the absolute value of binding energy $|BE| = mc^2 - E_0 \to mc^2$, its maximum possible value. In fact, we think this result is obtained in the context of an ill-defined system, uniquely on a pure mathematical basis.

From a physical point of view, we can see the coupling constant α is actually entangled with several fundamental constants, in particular the Planck constant, the velocity of the light, and the elementary electric charge. So, modifying α without caution can certainly lead to paradoxical physical results (e.g., letting α go to zero means that the charge does also; thus, there are no bound states and no *BE*).

There is another well-known example of changing a physical constant to obtain results: the non-relativistic limit of a relativistic theory can be obtained if one lets c tend to infinity, and thus the relativistic coefficient γ becomes 1 for any speed. However, as noted in [22] if doing this on the Dirac operator in an electro-magnetic field, one has to proceed carefully because of terms as such as mc^2, which would tend to infinity, and as the term $(e/c)\,\mathbf{A}$ that would turn off the vector potential $\mathbf{A}$ if c tends to infinity. Then the author is led to develop specific techniques and to define some concepts needed to account for the nature of the so-called *c-dependence* of the Dirac operators.

I-2. The wavefunction can have a singular point at the origin

This argument is rising in all known cases of EDO states with a 1/r Coulomb potential. The spatial part of solutions of the radial equation, in the most general form, has several factors:

- One factor is a decreasing exponential such that the wavefunction vanishes when $r \to +\infty$
- Another one is $\propto r^s$ with s a real number, due to the Coulomb potential
- A further one has polynomial form, possibly derived from confluent hyper-geometrical series

For the solutions called “anomalous”, the exponent s of the factor in r^s is negative, then the radial function $R(r) \to \infty$ when $r \to 0$ and the wavefunction $\psi(r,\theta,\varphi)$ does not obey a boundary condition.

Some authors of EDO solutions remove this trouble by saying that the classical expression of the central potential is a good approximation for the bound state of a single electron atom, but considering the nucleus as a mathematical point is an unphysical abstraction. In fact, the Coulomb approximation in $1/r$ of the central potential generated by the nucleus is suitable only if the electron is not too near the nucleus

At this point, many authors do not consider a non-singular potential and stop without further development of the anomalous solution. Others work on this subject by expressing corrected potentials in the close vicinity of the nucleus, as e.g. in [4]. We analyze this work in part II.

Moreover, we can see below that for the K-G case, the question of singularity can be resolved without modifying the potential.

I-3. The wavefunction can be ‘not square integrable’

If the wavefunction is not integrable, it cannot be normalized in the entire space. This case results essentially from the behavior of the wavefunction ψ at the origin and not for $r \to \infty$, thanks to the decreasing exponential. According to the spherical coordinates and the corresponding Jacobian, the norm of ψ is defined by $||\psi(r,\theta,\varphi)|| = \int|\psi|^2 \sin\theta\ r^2 d\theta\, d\varphi\, dr = \int|Y(\theta, \varphi)|^2 d\Omega \int|R(r)|^2 r^2\, dr$, where Ω is the solid angle. Since the spherical harmonics are normalized, one has only to verify that $\int|R(r)|^2 r^2 dr$ is finite, and this depends only on the behavior of $|R(r)|^2 r^2$ at the origin.

Here we can cite the work of Naudts [24], where an EDO state is found by using the Klein-Gordon (K-G) equation and the corresponding solution is square integrable. In his paper, the K-G equation has the following form:

$$(i\hbar\partial_t - V)^2\psi(r,t) + \hbar^2c^2\Delta\psi(r,t) = m^2c^4\psi(r,t) \tag{4}$$

Historically this equation was called *relativistic Schrödinger equation*.

We can note a time-dependence, because the author derived this equation from the time-dependent Schrödinger equation by introducing the relativistic formulation of the energy. This transformation was described in detail in [2]. We can note also, that the author considers only the case where the angular momentum is null: while expressing the Laplacian Δ in spherical coordinates, he eliminates the term involving the angular momentum operator, $L^2(1/r^2\hbar^2)$, and so the classical term in $l(l+1)$, representing the eigenvalues of $L^2/\hbar^2$, does not occur in his computation. By means of a suitable ansatz, the author finds a regular solution and an "anomalous" one. For this latter one, he obtains an electron total energy $E \sim mc^2\alpha \sim 3.73$ keV. So the binding energy is $BE \sim mc^2(\alpha - 1)$ -507.3 keV. He uses the following ansatz:

$$\psi(t,r) = e^{i/\hbar Et} r^{-l} e^{-r/r0} \tag{5}$$

Here the parameter denoted as l is not to be confused with angular momentum. As the author looks for solutions satisfying the hypothesis $l < 3/2$ and $r0 > 0$, the behavior of $|\psi(r,t)|^2 r^2$ at the origin ensures the square integrability of the wavefunction.

On another hand, as the deep orbit state corresponds to the plus sign in the solution $l = \frac{1}{2}(1 \pm \sqrt{1 - 4\alpha^2})$, we can see that the origin is a singular point for the wavefunction. Naudts argues against this problem by saying that the nucleus is not a point, but its charge is "smeared" over a distance of about 1fm. Solving the equation with a smeared out Coulomb potential would produce a solution not diverging at the origin, but with certain minor changes on the deep orbit state. We can add that, in the case of heavy nuclei, the regular solutions of the relativistic Schrödinger equation have also a singular point at the origin, because the coupling parameter $\gamma = Z\alpha$ is not "small" (e.g., for atom U, it is equal to ~ 0.45).

Another more subtle criticism concerns the well-known problem of the conservation equation: for the K-G equation, the density ρ is proportional to $\frac{\hbar}{2i\mathbf{m}c^2}(\psi^*\partial_t\psi - \psi\partial_t\psi^*)$ and cannot be considered as a probability density, because it can be negative [28], but it is interpreted as a charge density if taking into account the electromagnetic field in the conservation equation. Regardless, this question does not remove the interest in the EDO solution found by Naudts, and its square-integrability.

Finally we note two things:

- If the singular point at the origin (in the 'Coulomb' potential or the solutions) is suppressed, the wavefunction is automatically square-integrable.
- The square-integrability cannot be obtained for the Dirac equation in a pure Coulomb potential. This point is quickly proven by Naudts on a simplified form of radial Dirac equations.

I-4. The orthogonality criterion cannot be satisfied

The Hamiltonian, representing the total energy, has to be a Hermitian operator in order for its eigenvalues to be real. This implies the following condition: eigenfunctions corresponding to distinct values have to be orthogonal. In [25], de Castro examines the asymptotical behavior of the solutions of the non-relativistic Schrödinger, of the Klein-Gordon and of the Dirac equations, as functions of formal variations of the coupling constant α. We note that, for doing this, one could as well consider variations of $Z\alpha$, to cope with heavy nuclei.

He indicates the following conditions to obtain orthogonality:

- For the K-G equation: $(u_k^* (du_{k1}/dr) - u_{k1} (du_k^*/dr)) \to 0$ when $r \to 0$, where $u_k(r) = r R(r)$
- For the Dirac equation, a condition on the components *f, g*: $\left(f_k^* g_{k1} - f_{k1} g_k^*\right) \to 0$, when $r \to 0$

Then he obtains the following result:

Square-integrable solutions of the K-G equation satisfying the orthogonality criterion are such that for $\alpha \leq ½$, all the values of l (the angular momentum) are allowed. So, one can say that for the light atoms (including atom H and their isotopes), the orthogonality criterion is satisfied for l=0. On the other hand, for the Dirac case, the author indicates that only the regular solutions for the component functions *f, g* can satisfy the orthogonality. We can also note several works [26] [27] on self-adjoint extension of operators for potentials with singularity. In particular, the first cited work explicitly shows that, for the Klein-Gordon equation in the case of the pure Coulomb potential, the "singular" solutions satisfy the orthogonality condition and also satisfy the boundary condition: when $r \to 0$, $\lim u(r) = u(0) = 0$.

I-5. Consequences and recall on the first work of Maly and Va'vra on "DDLs"

With regards to the question above, we can see the Dirac equation has to be distinguished from the K-G equation. So, as all the problems mentioned are related to the singular point of the Coulomb potential, the anomalous solutions of Dirac equation require eliminating the singularity of this potential while considering a nucleus with finite dimension. Moreover, this is a more realistic hypothesis from a physical point of view. This is addressed in part II.

First we consider the specific works of Maly and Va'vra in [3] on deep orbits as solutions of the Dirac equation, named Deep Dirac Levels (DDLs), because they present the most complete solution and development available and include an infinite family of DDL solutions. In fact, they define DDL solutions for the electronic orbits of the hydrogen-like atoms, by means of the relativistic Schrödinger equation, and by the Dirac equation. Here we consider only hydrogen atoms. As this work has been already described in detail in [1] and yet more in [2], we focus on the Dirac equation and we recall only the results and the principal points of our analysis.

The Dirac equation was obtained by linearizing the classical relativistic energy-momentum relation $E^2 = \mathbf{p}^2c^2 + m^2c^4$ before translating the physical quantities into quantum operators.
So, the "free" Dirac equation has the standard following form:

$$(i\hbar\partial_t + i\hbar c\,\boldsymbol{\alpha}.\nabla - \beta mc^2)\,\boldsymbol{\Psi}(t,\mathbf{x}) = 0 \qquad (6)$$

where the momentum **p** was represented by means of the gradient differential operator and $\boldsymbol{\alpha}$ is the 3-vector of Dirac matrices. The Dirac equation is applied to the atom H and we consider only the bound states of the electron. In these conditions, the electron is subjected to an external electromagnetic field, in the form of the static Coulomb potential generated by a proton, and the potential energy is represented by $V = -\frac{e^2}{r} = -\alpha\frac{c\hbar}{r}$. Then, the Dirac equation in central Coulomb potential reads:

$$(i\hbar\partial_t + i\hbar c\,\boldsymbol{\alpha}.\nabla - \beta mc^2 - V)\,\boldsymbol{\Psi}(t,\mathbf{x}) = 0 \qquad (7)$$

1.5.1. Method used by the authors and results

The authors refer to and use the method developed by Schiff [28].
Here is the expression of the total energy of the anomalous solutions for atom H, very similar to the classical one for the regular solutions. The difference is the sign "minus" instead of "plus" between n' and the square root, at the denominator of the internal fraction:

$$E = mc^2\Big[1 + \frac{\alpha^2}{\left(n' - \sqrt{(k^2 - \alpha^2)}\right)^2}\Big]^{-1/2} \qquad (8)$$

In this expression, n' is the radial quantum number and k the specific angular Dirac quantum number.
In fact, the sign "minus" before the square root originates from the parameter $s = \pm (k^2 - \alpha^2)^{1/2}$ which appears during the process of solution of Dirac radial equation system. If $s > 0$, the obtained solutions are the "regular" ones; while, if $s < 0$, one obtains the "anomalous" ones.
The number n' can take any positive integer values 0, 1, 2 … while k can take any integer value $\neq 0$.
The authors yield computation results for values of the binding energy $|BE|$ as a function of quantum numbers n', k and the total quantum number n (denoted by conventional letters corresponding to regular orbitals). We can see the values of $|BE|$ are greater than 509 keV, and we can observe the following facts:

- The value of $|BE|$ increases when k increases

- The deep Dirac orbits levels (DDL) correspond only to the situation $n' = k$.
- Among the other cases, if $k > n'$, the authors indicate that the values correspond to “negative energy“ states,
- While if $k < n'$, the values correspond to energy levels similar to the “regular states”.

1.5.2. Analysis of the results

First, we can see there is infinity of DDL states: one for each value of k.

The same result is obtained by means of the relativistic Schrödinger equation, where the angular number is l.

- The relation $n' = k$ is very important, since it determines the DDL states.

In fact, it has a simple mathematical explanation. Indeed, we can see that if $n' = k$, the sub-expression D of the total energy E, $D = n' - (k^2 - \alpha^2)^{1/2}$ reads $D = k - (k^2 - \alpha^2)^{1/2}$, D becomes very small since $D \sim \alpha^2/2k$ and $E \sim mc^2\alpha/2k$. Then $|BE| \sim mc^2(1-\alpha/2k)$ and $|BE|$ is close to the rest mass energy of the electron, 511 keV.

We note a similar relation for the anomalous solutions of the relativistic Schrödinger equation, with an analogous mathematical explanation: the deep orbits appear only if $n' = l$.

Indeed, one has only to look at the concerned expression of the total energy:

$$E = mc^2[1 + \frac{\alpha^2}{(n' + \frac{1}{2} - [(l+\frac{1}{2})^2 - \alpha^2]^{1/2})^2}]^{-1/2} \tag{9}$$

One can see that $n' = l$ implies a drastic reduction of the denominator. This implies $E \sim mc^2\alpha/(2l+1)$, and thus $|BE| \sim mc^2[1-\alpha/(2l+1)]$.

- Moreover, one can see also that *Special Relativity is determining for the existence of EDOs*.

Indeed, the sub-term $s = -\frac{1}{2} - [(l+\frac{1}{2})^2 - \alpha^2]^{\frac{1}{2}}$ that occurs at the denominator, is in fact a parameter essential for choosing between the anomalous solutions and the regular solutions. It is in a root of a quadratic equation, $s(s+1) - l(l+1) - \alpha^2 = 0$, which appears when solving the relativistic Schrödinger equation. The other root, $s = -\frac{1}{2} + [(l+\frac{1}{2})^2 - \alpha^2]^{\frac{1}{2}}$, leads to regular solutions.

Nevertheless, we must emphasize that, in the *non-relativistic case*, a similar quadratic equation, very close to the previous, appears: $s(s+1) - l(l+1)$. We can see that is this last case, the solutions no longer contain α^2 and are simple integer numbers: $s = l$ gives the regular case, and $s = -(l+1)$ the anomalous one. In this latter case, it is no longer possible to apply the ‘recipe’ that discriminates the EDO from the anomalous solutions, because $n' = l$ would lead to a null denominator in the expression of the energy of anomalous solutions, similar to the expression written above, but without the term α^2. So, we can say that it is not possible to find EDO in this case.

Now we return to the Dirac solutions, the DDLs, and we consider the relation $|BE| \sim mc^2(1-\alpha/2k)$ written above. We can see that $|BE|$ *increases when k increases*, as observed on the tables of Maly and Va’vra. Of course, it’s the same thing in the Schrödinger case. We note that *this progression is opposite to that of the one of the regular states*. By seeing this, one can suppose that the electron orbitals are progressively closer to the nucleus when k increases. This fact is not explicitly mentioned in [3] or in their next work [4], but it can be deduced from a sentence in the latter paper.

Here we prove it by direct computation of the mean radius of the DDL orbital, as explained in the next part, devoted to our work on [4].

- To understand why the case $k > n'$ corresponds to negative energy states (compatible with Dirac equation), it is necessary to know the process of solving the radial equation. In fact, this can be deduced from the following relation (23) in [3], or [28, p.486]: $2\alpha(s + n') = (2E\gamma)/\hbar c$. So E has the sign of $(s + n')$, and as $s < 0$, we have $s + n' \sim n' - k + (\alpha^2/2k) \leq -1 + (\alpha^2/2k) \sim -1$, since $k > n'$ and $\alpha^2/2k$ is very small.
- When $k < n'$, one can observe from the algebraic expression of E above, that for any couple (n', k) satisfying this inequality, E is very close to the energy of a *regular level* corresponding to a value of the principal quantum number N taken equal to $n' - k$.

We called these states, “pseudo-regular” states, because the levels correspond to regular levels, while the wavefunctions have the form of anomalous solutions, since they are determined by a negative parameter s.

II. The deep orbits (DDL) obtained as solutions of the Dirac equation with a corrected potential near the nucleus

After their first paper [3] on the computation of the DDL levels, the authors continued their study with a second paper [4] on the solutions of Dirac equation for hydrogen-like atoms, where they consider that the nucleus is not point-like and the Coulomb potential inside the nucleus is finite at $r = 0$.
For doing this, they start with another method (Fluegge [29], p.195) for the Dirac equation solution, than the one of Schiff [28] used in the first paper. As usual, the solution of Dirac equation can be represented, in central field, by a 4-D vector with two 2-D components, and each component is the product of one radial function with a 2-D spherical spinor.
Then the process of separating the variables leads in general to a system of coupled first order differential equations on both radial functions $f(r)$ and $g(r)$. The exact form of this equation system is dependent on some choices made in the variable separation process, but these different forms are very similar. Here is the system used in [29], where j is the angular quantum number corresponding to the total angular momentum **J** operator**,** sum of the orbital momentum and the spin:

$$\begin{aligned} g' + \frac{j+\frac{3}{2}}{r} g - i\frac{E - V(r) - mc^2}{\hbar c} f = 0 \\ f' - \frac{j-\frac{1}{2}}{r} f - i\frac{E - V(r) + mc^2}{\hbar c} g = 0 \end{aligned} \tag{10}$$

One can replace j by putting $k = j + ½$.
In the method of solution of Fluegge (p.195), the equation system is transformed into a 2^d order differential equation, a Kummer's equation. The general solutions of this equation take the following form, with confluent hyper-geometrical series requiring suitable convergence conditions:

$$\begin{aligned} g &= \frac{1}{2} C r^{s-1} e^{-r/a} \left\{ {}_1F_1\left(s+p, 2s+1; 2\frac{r}{a}\right) - \frac{s+p}{k+q}\, {}_1F_1\left(s+p+1, 2s+1; 2\frac{r}{a}\right) \right\} \\ f &= -\frac{i}{2\mu} C r^{s-1} e^{-r/a} \left\{ {}_1F_1\left(s+p, 2s+1; 2\frac{r}{a}\right) + \frac{s+p}{k+q}\, {}_1F_1\left(s+p+1, 2s+1; 2\frac{r}{a}\right) \right\} \end{aligned} \tag{11}$$

Here, ${}_1F_1$ is a classical notation for a precise class of hypergeometric series [30]
The parameters a, μ are usual parameters including the energy E, p and q are defined by means of μ. These parameter are used to simplify the writing and to have equations with pure numerical variables. It is unnecessary to write out their expression, because our discussion will focus on the solutions “inside” the nucleus. The parameter s is determined by means of the equation system, for $r \to 0$, that gives $s = \pm (k^2 - \beta^2)^{1/2}$ where $\beta = Z\alpha$ and α is the coupling constant. Note that the expressions of f and g depend on k and s. We know that DDL solutions result when a negative s is chosen.

-1. Determining the solutions inside the nucleus

-1.1. The Matching radius and the continuity condition
While considering the nucleus has finite dimension, the authors choose a finite specific potential inside the nucleus and then look for the wavefunctions inside the nucleus. The chosen potential is derived (by adding a constant β0) from the Smith-Johnson potential, corresponding to a uniformly distributed spherical charge, whose expression is the following:

$$V(r) = -\left[\frac{3}{2} - \frac{1}{2}\left(\frac{r^2}{R_0^2}\right)\right] \frac{Ze^2}{R_0} + \beta 0 \tag{12}$$

In fact, we consider β0 has to be null since, in the case $\beta 0 \neq 0$ the total potential from 0 to $+\infty$, built by connecting it with the Coulomb potential, would be discontinuous at $r = R_0$.
R_0 is the “matching” radius, i.e. a radius near the nucleus such that the following rules are applied:

- For $r < R_0$, the potential is $V(r)$ and the wave-functions solutions are the “inside” ones, noted f_i and g_i. Here we consider $Z = 1$ (for hydrogen atom).

- For $r > R_0$, the potential is the standard Coulomb potential and the wave-functions solutions are the outside" ones, f_o and g_o, as noted.

- The inside and outside solutions have to verify the continuity condition, i.e. $g_i(R_0) = g_o(R_0)$ and $f_i(R_0) = f_o(R_0)$. This condition is sufficient, because the Dirac equation is first order differential in the space coordinates.

As a result of some criticism about the matching conditions at the boundary, we thought that it was necessary to verify the method and the results of the computation indicated in [4].

First, there is the question of the choice of R_0. As this value is not explicitly given in their paper, we chose the value R_0 =1.2 fm as in the work of Deck et al. [31], where the authors use the formula $R_0 = 1.2\,A^{1/3}$, A being the mass number. On Fig.2 in [4], representing the curve of the Electron Density of a DDL atom H for k=1, one can estimate that the peak is at a value of the radius slightly > 1 F but < 1.2 F. The authors say that this peak corresponds to the nucleus radius. One will observe that it corresponds to the value of the matching radius (see results below in section 2.1). In fact, one has to choose a value of R_0 close of the charge radius Rc of the nucleus but slightly greater than Rc: one supposes that in the close neighborhood of the nucleus, the strength of the electric field no longer increases. So, for atom H, as the proton has $Rc \sim 0.875$ F in CODATA 2014 [32] or in [33], one can reasonably choose 1F < R_0 < 1.25 F.

We have performed the computation particularly for atomic H, but if we consider atomic D, the previous empirical formula would give $Rc \sim 1.51$ F. Nevertheless, in modern tables cited above, we can see that $Rc \sim 2.14$ F, so we could choose 2.26 F< R_0 < 2.5 F. We will see further how the results change when we modify the matching radius R_0.

-1.2. Ansatz used for finding the "inside" solutions

The choice of an ansatz is a very important element for finding the solutions f_i and g_i of the initial system of radial equations. Moreover, its expression is determined to satisfy the continuity condition.

In their paper [4], the authors put solutions in the following form:

$$g_i = Ar^{S_i-1}\, G_2(r) \qquad (13)$$
$$f_i = \mathrm{i}Br^{S_i-1}\, F_2(r)$$

where $G_2(r)$ and $F_2(r)$ are power series, i.e.

$$G_2(r) = a_1 r + a_2 r^2 + a_3 r^3 + \dots \quad \text{and} \quad F_2(r) = b_1 r + b_2 r^2 + b_3 r^3 + \dots \qquad (14)$$

We note that one can eliminate the imaginary number "i" coefficient from the definition of the inside function f_i as from the outside function f_o, by posing $f_{o1} = -\mathrm{i}f_o$ and $f_{i1} = -\mathrm{i}f_i$ in the equation system. We consider from here, that f_i and f_o no longer contain "i" in their respective coefficients.

Next the equation system leads to couples of interdependent recurrent formulas for computing the coefficients of both power series $G_2(r)$ and $F_2(r)$. As usual, one has to annul the coefficients of the successive powers of r in the unfolded polynomials. But it seems that the information given in the paper is incomplete, because when unfolding both recurrence relations (4, p.61), the coefficient A automatically disappears and the polynomials $G_2(r)$, $F_2(r)$, take the following forms $G_2(r) = Bb_1\, G(r,k)$, $F_2(r) = Bb_1 F(r,k)$, where $G(r,k)$ and $F(r,k)$ are expressions depending only on the radius r and the quantum number k. Then, when trying to satisfy the continuity condition with the couple of equations $\{g_i(R_0) = g_o(R_0)\ ,\ f_i(R_0) = f_o(R_0)\}$, and taking into account that these equations have to be satisfied for any *fixed* value of k, one gets a couple of linear equations in the form $\{G_i = K\, G_o\ ,\ F_i = K\, F_o\}$ where $K = C/Bb_1$ is the only unknown and G_i, G_o, F_i, F_o are four constants $\neq 0$ and such that $G_i/G_o \neq F_i/F_o$. Of course, this system has no solution.

We think that useful information was in another paper of the same authors, referenced as "to be published" but which unfortunately was not published. In fact, the disappearance of A is due to the starting couple of recurrent relations:

$$\{(k + s_i + 1)\, a_1 A = 0\ ,\ (-k + s_i + 1)\, b_1 B = 0\} \qquad (15)$$

This leads to two possible choices for having convergence at $r = 0$:

for $k<0$, $s_i = -k - 1$, $b_1 = 0$ and $a_1 \neq 0$, which leads to the disappearance of B

or for $k>0$, $s_i = k - 1$, $a_1 = 0$ and $b_1 \neq 0$, which leads to the disappearance of A.

To resolve this problem, the only solution is to *add a further parameter* in the power series, in such a way that it could not be merged with the multiplicative coefficient B (choice $k>0$). For doing this, we consider the following more complex power series for $G_2(r)$ and $F_2(r)$:

$G_2(r) = a_1 (\lambda r) + a_2 (\lambda \mathrm{r})^2 + a_3 (\lambda r)^3 + \ldots$ and $F_2(r) = b_1 (\lambda r) + b_2 (\mathrm{r})^2 + b_3 (\lambda r)^3 + \ldots$

Of course, one must not confuse this change with a scale change for r, because r remains the only variable for derivative in the differential Dirac equations, and the recurrence relations are rather similar to the ones of [4] but including the parameter λ in a simple way. They have the following form:

$$a_n (\lambda (s_i+k+n)) = (B/A) (K_1 b_{n-1} + (\beta_2 b_{n-3})/\lambda) \qquad (16)$$
$$b_n (\lambda (s_i-k+n)) = (A/B) (K_2 a_{n-1} - (\beta_2 a_{n-3})/\lambda)$$

where K_1 and K_2 are parameters depending on the (total) energy E and on constant parameters β_1, β_2 used to write the expression of the potential inside the nucleus:

$$V = \hbar c(-\beta_1 + \beta_2 r^2) \qquad (17)$$

We unfold the recurrent relations with the choice $k>0$, and we obtain the expressions of g_i and f_i in the form of two polynomials in λ and r. As indicated by the authors, we can limit the maximum powers to 6 (5 in their paper) in the initial polynomials $G_2(r)$ and $F_2(r)$, since $r < R_0$ is very small and one can neglect higher order terms. The progression of powers with k is the following:

-For $k = 1$, the polynomial f_i has degree 4 in r and includes only even power terms while g_i has degree 5 in r and includes only odd power terms.

-When k changes into $k+1$, the degrees in r increase by 1 and the parities of the power terms occurring in the respective polynomials alternate.

- But, for any k, the maximal degree of λ remains constant and equal to 2.

More precisely, for any fixed $r > 0$, g_i and f_i can always be factorized into the form $(a \lambda + b) \lambda$. This form is very useful because it always ensures a solution of the matching problem for the inside and outside wavefunctions at $r = \mathrm{R}_0$. Indeed, the equations of continuity condition $\{g_i(R_0) = g_o(R_0), f_i(R_0) = f_o(R_0)\}$ lead to a couple of pseudo-quadratic equations with two unknowns λ and C (the multiplicative coefficient common to both outside wave-functions) in the following form, where the coefficients a, b, a', b', c, c'(depending on k and on R_0) are always $\neq 0$ and are taken >0:

$$(a \lambda - b) \lambda - c\, C = 0$$
$$(a' \lambda + b') \lambda + c' C = 0 \qquad (18)$$

This system is reducible into two linear equations. A plus sign occurs before c' because f_o is always a negative function while g_o is a positive one. Moreover, a minus sign occurs before b, and we have $c >> c'$ and $b' >> b$: this can be showed by recurrence on k. In these conditions, we have $ac'+a'c \neq 0$ and $bc'-b'c \neq 0$, what allows to obtain $\lambda \neq 0$, then $C \neq 0$ by a similar reasoning. So, the system has a non-trivial solution which can be used (apart from the trivial solution $\lambda = C = 0$).

-1.3. The question of orthogonality and the boundary condition

If we consider a couple of "inside" functions (g_i, f_i), the term of minimal degree of the polynomial g_i is k and for f_i it is $k-1$. So, in the formula used to verify the *orthogonality criterion* (Part I, section 4), $\left(f_k^* g_{k1} - f_{k1} g_k^*\right) \rightarrow 0$ when $r \rightarrow 0$, the expression to be considered is a polynomial P having a term of minimal degree $k + k1-1$ and thus, for any $k > 0$, P does not contain any constant term. We can deduce that *the corresponding global solution satisfies the orthogonality condition*.

Next, if we look at the boundary conditions, expressed by $g_i \rightarrow 0$ and $f_i \rightarrow 0$ when $r \rightarrow 0$, we can see this property is verified for any $k > 1$.

-2. Results obtained by computing the wavefunctions and consequences

While having the expressions of the couple of whole wave-functions from $r = 0$ to $+\infty$, built by connecting g_i to g_o and f_i to f_o, one can obtain important information on the electron orbital.

As in the cited work, we use the Electron Density (ElD) expression, which is the *radial probability density* defined by the wavefunctions, for computing the normalization constant and next to compute the mean radius $<r>$ of the orbital for different values of the quantum number k. We would like obtain a formal expression of <*r*> as function of *k*. Unfortunately the expressions of the wavefunctions are very cumbersome, especially the expression for the outside functions including hyper-geometrical series. Furthermore, the last step is an integral. Nevertheless, while numerically computing <*r*> for several progressive values of *k*, one can observe the corresponding progression of <*r*> and even estimate the limit for very great *k*. Moreover, by modifying different parameters, such as the value of the matching radius, the degree of the initial polynomial of the ansatz, or the form of the nuclear potential, one can observe if and how changes in these parameters affect the orbitals, and thereby deduce a kind of "mathematical stability" of the orbitals.

- 2.1. Values of the mean radius, with matching radius $R_0 = 1.2$ F and for different values of *k*.

The value of the mean radius is an essential parameter for the LENR, since the range of the strong nuclear force is order of femto-meters (fm or F) and quickly decreases at distances > ~3 to 5 F. The mean radius of electron orbital determines the "size" of the atom and the value of the repulsive radius of an atom. This radius can be estimated approximately [4] to the value of *r* where ElD drops to 1/10 of its peak value.

The computation process is the following:

- For given *k*, to compute the functions g_i, g_o, f_i, f_o
- Next to compute the parameters, λ and *C*, for satisfying the continuity condition, as described above
- To insert the value of λ into the previous expressions of g_i, f_i and replace the parameter *C* by its value into the expressions of g_o, f_o
- To consider the Electron Density of the "outside" functions $ElDo = 4\pi\, r^2(|f_o|^2+|g_o|^2)$ and the ElD of the "inside" functions $ElDi = 4\pi\, r^2(|f_i|^2+|g_i|^2)$, and to compute the normalization constant *N* with the following formula:

$$1/N = [\int_0^{R0} ElDi\, dr + \int_{R0}^{+\infty} ElDo\, dr\,] \tag{19}$$

- Finally, to compute the mean radius with the following formula:

$$<r> = N\,[\int_0^{R0} r\, ElDi\, dr + \int_{R0}^{+\infty} r\, ElDo\ \ dr\,] \tag{20}$$

Doing this, we obtained the following values:

- $k = 1$, $<r> \sim 6.62$ F
- $k = 2$, $<r> \sim 1.65$ F
- $k = 3$, $<r> \sim 1.39$ F
- $k = 10$, $<r> \sim 1.226$ F
- $k = 20$, $<r> \sim 1.207$ F

1. As a first consequence of this result, we observe that we obtain values of *the same size order* as those in [4], while we used *a method which is likely different* (for computing the inside functions). So, we have a good confirmation of the prior results. Those authors indicate explicitly the value 5.2 F for the DDL atom H for $k = 1$ and their matching radius seems to be slightly >1F but <1.2F. They say further, "The main point of this section is that the size of atoms with all electrons on the DDL levels can be very small. Under some conditions ($l > 10$) such atoms (H) with all electrons on the DDLs might participate in the secondary nuclear reactions," to be related to a previous phrase: "it is well known that the short-range nuclear forces are acting at a distance of 3 to 5 F."

2. With our computation results, we can see *the mean radius decreases when k increases*. This was suggested by those authors (by the cited phrase above) and it is consistent with the fact that the binding energy in absolute value $|BE|$ increases when *k* increases [1].

3. Finally, we can see also that, after an abrupt fall at the beginning of the progression, the value of the radius asymptotically tends to the value of the matching radius 1.2 F. In figure 3, we plot the curves of the normalized ElD for *k*=1, 2 and 3.

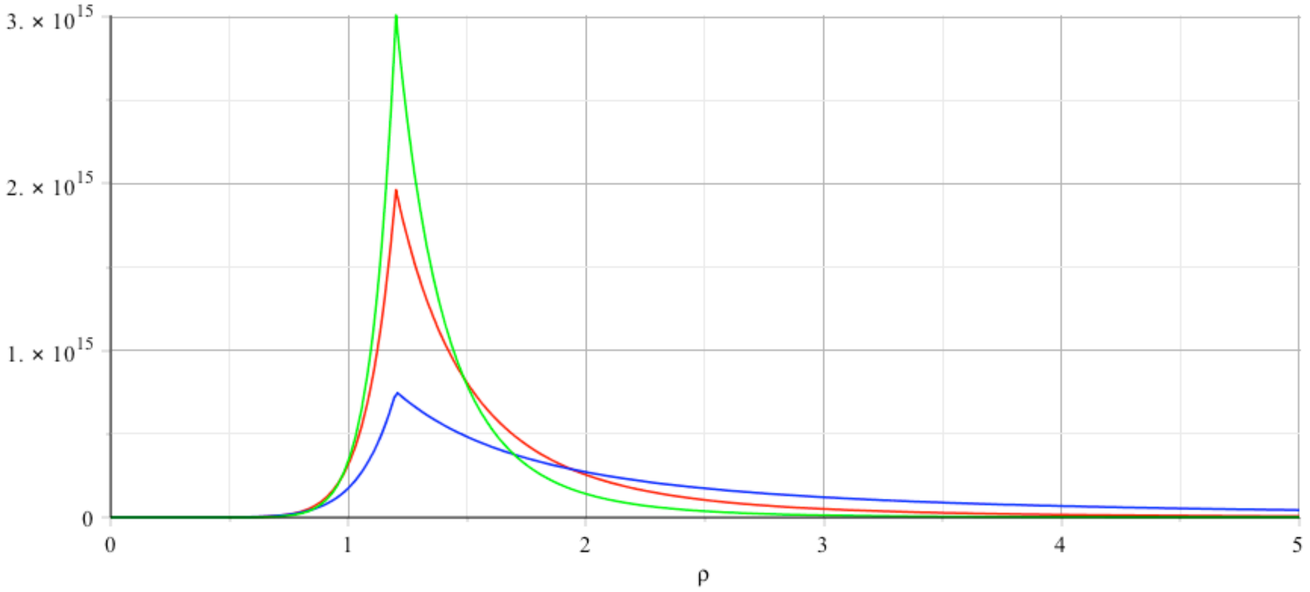

Fig.3. Normalized ElD, for *k*=1 (blue), *k*=2 (red); *k*=3 (green). The radius ρ is in F.

2.2. Values of the mean radius, obtained when increasing the precision of the inside functions.

Now we give results obtained when starting from polynomials $G_2(r)$ and $F_2(r)$ until degree 8. Of course, the method of computation is the same, but this time the polynomials g_i, f_i have degree 3 in λ. But for any fixed $r > 0$, they can always be factorized into the form $(a\,\lambda^2 + b\,\lambda + c)\,\lambda$.

The verification of the continuity condition leads to a couple of equations of the following form, where the coefficients a, b, c, d, a', b',c',d' are ≠0 and are taken >0:

$$\begin{aligned}&(a\,\lambda^2 + b\,\lambda - c)\,\lambda - d\,C = 0\\&(-a'\,\lambda^2 + b'\,\lambda + c')\,\lambda + d'\,C = 0\end{aligned}\qquad(21)$$

This system can be reduced into a quadratic equation and a linear equation. To rigorously prove it has always a (non-trivial) solution is rather tedious. In fact one has to choose between two solutions very near in absolute value, but with roots λ of opposed signs.

In any case, the values computed for the mean radius are:

- $k = 1$, $\langle r\rangle \sim 5.91$ F
- $k = 2$, $\langle r\rangle \sim 1.51$ F
- $k = 3$, $\langle r\rangle \sim 1.305$ F
- $k = 10$, $\langle r\rangle \sim 1.204$ F

One can observe that the values are slightly smaller than the ones obtained with polynomials of degree 6, but the absolute and relative shifts are monotonically smaller with k increasing

- $k = 1$, $\Delta\langle r\rangle \sim -0.7$ F , $\Delta\langle r\rangle/r \sim -0.10$
- $k = 2$, $\Delta\langle r\rangle \sim -0.14$ F, $\Delta\langle r\rangle/r \sim -0.08$
- $k = 3$, $\Delta\langle r\rangle \sim -0.085$ F, $\Delta\langle r\rangle/r \sim -0.06$
- $k = 10$, $\Delta\langle r\rangle \sim -0.022$ F, $\Delta\langle r\rangle/r \sim -0.017$

Thus, the new series of values converges to the previous one, and one can reasonably assume that both series of values converge to the same limit, the matching radius ~1.2 F

-2.3. Values of the mean radius obtained when modifying the value of the matching radius

To see what happens if we change the value of matching radius, we recalculate the mean radius for a value distinctly smaller that 1.2 F, by letting R_0 = 0.78 F. As above, the values of the mean radius become smaller (with increasing k) and tend to 0.78 F. So we obtain the following values:

- $k = 1$, $\langle r\rangle \sim 4.6$ F
- $k = 2$, $\langle r\rangle \sim 1.07$ F
- $k = 3$, $\langle r\rangle \sim 0.9$ F
- $k = 10$, $\langle r\rangle \sim 0.797$ F

Of course, this was only an abstract exercise since this value of R_0 = 0.78 F is unrealistic, from a physical point of view, for atomic H (but it is perhaps not unrealistic if a DDL electron is present). On the other hand, if we consider a nucleus heavier than of H, as e.g. Li6, the mean radius will be greater.

So, as for Li6, we have Rc ~2.59, we can reasonably choose e.g. R_0 = 2.8 F. With this value for R_0, the computation yields the following results confirming our model:

- k=1, <r> ~ 13.4 F
- k=2, <r> ~ 3.84 F
- k=3, <r> ~ 3.25 F
- k=4, <r> ~ 3.06 F
- k=10, <r> ~ 2.85 F

-2.4. Values obtained by changing the nuclear potential

Until now, we performed our computations while considering that the potential corresponds to a uniformly distributed spherical charge. Its expression is the following:

$$V(r) = -\left[\frac{3}{2} - \frac{1}{2}\left(\frac{r^2}{R_0^2}\right)\right]\frac{Ze^2}{R_0} \quad \text{, with } Z = 1 \tag{22}$$

This potential was introduced into the "inside" functions fi, gi by means of the following formula :

$$V(r) = \hbar c(-\beta 1 + \beta 2\, r^2), \quad \text{where } \beta 1 = (3/2)\, \alpha/R_0 \text{ and } \beta 2 = (1/2)\, \alpha/R_0^3 \tag{23}$$

Now we consider a further parameter $\varepsilon \geq 0$ and we put $\beta 1' = ((2+\varepsilon)/2)\, \alpha/R_0$ and $\beta 2' = (\varepsilon/2)\, \alpha/R_0^3$.

We can see that

- If $\varepsilon = 1$, we obtain the previous potential $V(r)$
- If $\varepsilon = 0$, we obtain a constant potential, equal to the value of the Coulomb potential at $r = R_0$.
- If ε has a very small value, the potential is almost constant, but it is more realistic from a physical point of view than a strictly constant potential.

We plot (figure 4) the previous form of potential defined from 0 to $+\infty$ by the following expression:

$Pot(r)$: {if r < R_0 then $Pot(r) = V(r)$, if $r \geq R_0$ then Pot(r) = $\alpha c\hbar/r$}

And we plot (figure 5) the curve of the derivative $dP(r)/dr$.

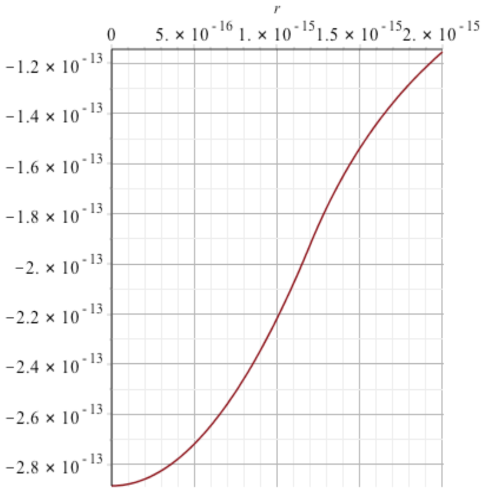

Fig.4. $Pot(r)$ on interval [0F, 2F]

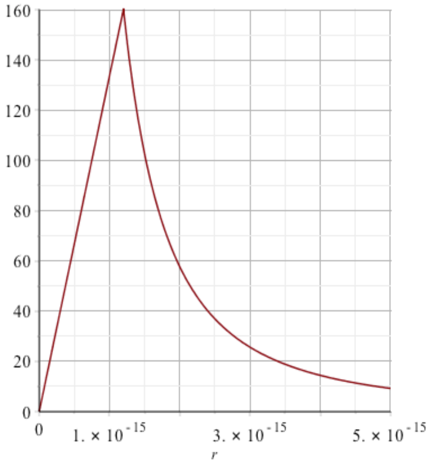

Fig.5. Derivative of $Pot(r)$

In figure 4, we can observe the inflection point at r = 1.2 F (the matching radius). The derivative (figure 5) is continuous, but the second order derivative is discontinuous at the inflection point

Now, we consider the modified nuclear potential $V_\varepsilon(r) = \hbar c(-\beta 1' + \beta 2' r^2)$ and the potential Pot_ε defined by the following expression: $Pot_\varepsilon(r)$ = {if $r<R_0$ then $Pot_\varepsilon(r) = V_\varepsilon(r)$, if $r \geq R_0$ then $Pot_\varepsilon(r) = \alpha c\hbar/r$ }. We plot this potential on figure 6, by taking $\varepsilon = 10^{-1}$ to better see its slight curvature and the previous potential $Pot(r)$. In figure 7, we plot only $Pot_\varepsilon(r)$ with $\varepsilon = 10^{-5}$.

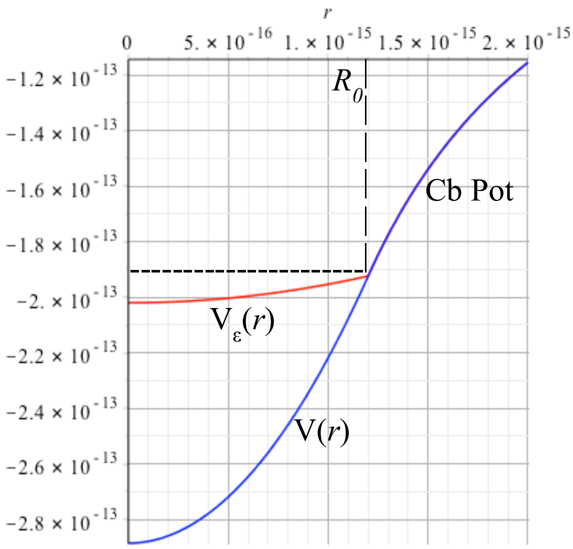

Fig.6. Pot(*r*) and *Pot*$_\varepsilon$(*r*) with ε = 10^{-1}

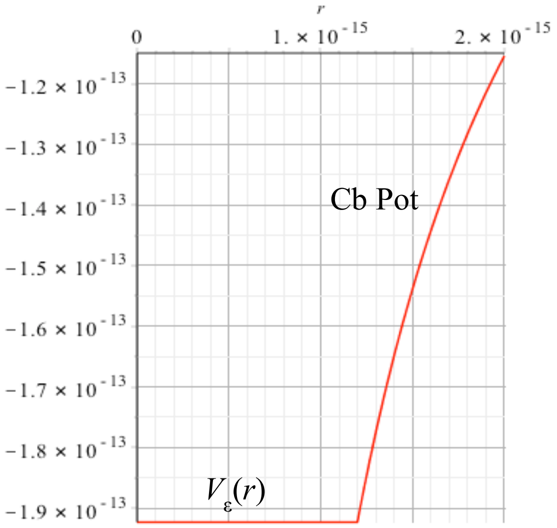

Fig.7. *Pot*$_\varepsilon$(*r*) with ε = 10^{-5}

Of course, in figure 6, both curves are merged for $r > R_0$. In figure 7, we can see that, with very small ε = 10^{-5}, the curve is practically flat for $r < R_0$ and the potential is almost constant. Using the flexible potential *Pot*$_\varepsilon$, instead of directly using a constant potential, has two advantages: we can easily try intermediate forms of potential and, with a very small ε, we obtain an almost constant potential.

The results with *Pot*$_\varepsilon$ are the following:

- $k = 1$, $<r> \sim 6.62$ F
- $k = 2$, $<r> \sim 1.65$ F
- $k = 3$, $<r> \sim 1.39$ F
- $k = 10$, $<r> \sim 1.226$ F
- $k = 20$, $<r> \sim 1.207$ F

We observe the same results as with the initial potential *Pot*(*r*). Thus, the mean radius is insensitive to the internal potential, but strongly dependent on the choice for matching radius. While this choice appears arbitrary, it may be uniquely determined by the Dirac equations solutions. This is future work.

- 3. Trying a process for increasing the dependence of the inside solutions on the nuclear potential

Finally, on account of a subtle criticism [31] about some lack of dependence of the solutions on the nuclear potential, we began to try a special resolution process.

In fact the outside functions are fully dependent on the Coulomb potential. But the inside functions are not very dependent on the nuclear potential *V*(*r*), because they involve DDL energy value *E* included in the energy parameters K_1 and K_2 in the recurrent relations (16) used to define the inside functions.

Indeed, we have $K_1 = [(mc^2 - E) / \hbar c] - \beta_1$ and $K_2 = [(mc^2 + E) / \hbar c] + \beta_1$, where β_1 is a coefficient included in the definition of the nuclear potential $V(r) = \hbar c(-\beta 1 + \beta 2\ r^2)$, while the second coefficient β2 is included in the recurrent relations (16).

So the general expression of the inside functions depends on *V*(*r*), but it depends also on *E* and thus on the Coulomb potential. So, it depends at once on *V*(*r*) and on the Coulomb potential.

In these conditions, we first do the following computation:

For fixed *k* and for a given value of the mean radius $<r>$ computed as previously, we compute an approximate mean value of the binding energy, by using the relativistic formulas of the potential energy (in absolute value) $Epot = -\gamma m v^2$, the one of the kinetic energy $KE = (\gamma\text{-}1)mc^2$, and by supposing that *Epot* is equal to the Coulomb potential energy, since the electron is outside the nucleus; next we compute the total energy $E' = mc^2 + KE - |Epot|$.

Doing this, we find that $E' \neq E$.

Then we try the following computation process, for “injecting more dependence” on the nuclear potential into the computation of the solutions:

- to "inject" E' in the global solution (g_iUf_i, g_oUf_o) by replacing E by E' in all the energy parameters of the radial equations,

- to compute the new mean radius $<r'>$, by using the process described in 2.1.

- if $<r'> \sim <r>$ on three digits, then we stop the process, else we iterate it.

Doing this, we obtain a surprising result: for any fixed $k > 1$, the process can stop by the first cycle. We list the following values of the binding energy (in absolute value) as function of k , corresponding to the values of the mean radius $<r>$ and computed as indicated above:

- $k = 2$, 275 keV, for $<r> = 1.65$ F
- $k = 3$, 301 keV, for $<r> = 1.39$ F
- $k = 10$, 320 keV, for $<r> = 1.22$ F

As $<r>$ tends to 1.2 F when k tends to $+ \infty$, we can suppose that $|BE|$ tends to a value ~ 323 keV. On account of these results, we *conjecture that these values are the actual values of the DDL binding energy for the corrected potential*, instead of the values given by the formula (8), which are greater than 509 keV.

For the case of $k = 1$, as $<r> = 6.62$ F, we have an important gap, in comparison with the values for $k > 1$. So, the computation process does not converge at the first cycle, but the values of the radius computed at the successive cycles seem to approximatively have the behavior of geometrical series, and to converge to a value ~ 12 F, that would give |BE| ~ 56.5 keV.

Conclusion about the new results, open questions, future paths.

The direct computations of the mean radii of the DDL orbitals yield the following results:

- First, we have an important result about the behavior of the orbitals as function of the angular quantum number k, which for the DDLs is equal to the radial number usually denoted by n':

When k (and thus n') increases, the mean radius $<r>$ decreases, which behavior is inverse of the classical orbitals. But this result is totally consistent with the fact that the binding energy $|BE|$ increases in absolute value when k increases, or equivalently that the total energy E decreases when k increases: this result was already noted in [1] and can be deduced from the tables of [3]. We can also observe it by noting that the $E \sim mc^2(\alpha/2k)$. A possible reason for this 'inversion' is that only the deep orbits 'see' the repulsive barrier, imposed by centrifugal forces at small r, as significant.

- Next, we can see that the value of $<r>$ asymptotically tends to a finite value $\neq 0$, and more precisely it tends to the value of the matching radius R_0. So, the orbitals converge when k increases and they accumulate in a spherical shell of radius $rlimit \sim R_0$ and $rlimit > R_0$. We can deduce that, for large values of k, the orbitals are no longer distinguishable. On the other hand, as this limit depends on the chosen matching radius, one could say that the determination of the orbitals depends on arbitrary elements. Nevertheless we can argue that the matching radius cannot be arbitrary, as highlighted in section II.1.1: one has to choose a value of R_0 close of the charge radius Rc of the nucleus, but slightly greater than Rc. As we do not yet know a more precise criterion for this choice, there remains some degree of incertitude as is usual in Quantum Mechanics.

- Finally, apart from the dependence on the matching radius, which is expected from a physical point of view, the values of the mean radius and especially their asymptotic behavior, seem rather independent of the precision of the functions inside the nucleus and of the chosen nuclear potential.

Open questions about the DDL orbitals include, in particular, the following ones:

- Is there really coherence between the energies of the DDL levels and the values of mean radius as herein computed for the orbitals? For resolving this question, we are presently working on a convergence method, starting from the value of DDL levels energies and inputting some dependence on R_0 and the nuclear potential into the computation, in order to reach energy values consistent with the corrected potential.

- What are the shapes of these orbitals?

In principle, their angular part should correspond to the classical spherical harmonics, as solution for the 2-D spherical spinors. The condition $k = n'$ could also give an indication for this question. Nevertheless, we can note that the radial wavefunctions of the DDLs have a behavior completely different from the classical atomic orbitals. For example, these latter ones have a number of zeros (radial nodes) equal to n', while the former ones have no radial node. So the question is: have the angular solutions associated with the DDLs a number of nodal planes corresponding to k?

- In the same vein, we can ask if the angular momentum is actually increasing with k, as it is the case in the regular solutions. But, as the progression of the DDL mean radii is the reverse of the one of the regular solution, has this reverse progression an influence on the progression of the angular momentum? According to the fact the DDL radii approach a limit, where they accumulate in a very small volume, and on account of the Heisenberg uncertainty relation, can we suppose that the angular momentum vector fluctuates in all directions for large k**,** so that the time-integrated orbitals could be spherical.
- Concerning the condition $k = n'$, which mathematically determines the DDL states among the anomalous solutions, the question remains to confirm the physical reason this relation yields the DDL states.
- How can we interpret the theoretical existence of pseudo-regular solutions deduced from the relation $k < n'$ (see 1.5.2.), i.e. wavefunctions corresponding to a negative s, but with energy values close to "regular" ones ?
- Special relativity seems decisive for finding DDLs solutions. Why?
- DDLs are in an extreme EM field. Can we expect a strengthening of special known effects?

Concerning the determination of the Dirac wavefunctions in a modified Coulomb potential without singularity, the best method could be a direct numerical computation of eigenfunctions of the Dirac operator with this potential. Because of the very great difficulty of such a computation method, we can rather envisage various semi-numerical and perturbation methods taking into account some magnetic properties like the ones indicated at the end of the introduction, which also suppose a repulsive core near the origin.

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