



Research Article

Relativity and Electron Deep Orbits of the Hydrogen Atom

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Abstract

This work continues our previous works 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 Electron Deep Orbits (EDOs). In a first part we quickly recall the known criticism against the EDO and how we face it. In particular, a solution to fix all problems is to consider a modified Coulomb potential with finite value inside the nucleus. For this reason, we deeply analyzed the specific work of Maly and Va'vra on deep orbits as solutions of the Dirac equation, with such a modified Coulomb potential without singular point. Then, by using a more complete ansatz, we made numerous computations on the wavefunctions of these EDOs, allowing to confirm the approximate size of the mean radii $\langle r \rangle$ of orbits and to find further properties. Moreover, we observed that the essential element for obtaining deep orbits solutions is special relativity. At a first glance, this fact results from an obvious algebraic property of the expression of energy levels obtained by the relativistic equations. Now, a comparative analysis of the relativistic and of the non-relativistic Schrödinger equation allows us to affirm that Special Relativity leads to the existence of EDOs because of *the non-linear form of the relativistic expression* for the total energy, which implies a relativistic non-linear correction to the Coulomb potential.

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1. Introduction

With the quantum equations habitually used in the literature for computing the bound states of the H atom, we note that there is, in the relativistic form, 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 because of its singularity at $r = 0$.

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

- (1) The relativistic equations can predict EDOs with a mean radius of order femto-meter; whereas the normal non-relativistic equations do not. We give a simple mathematical reason for this fact.
- (2) With an EDO having a mean radius of order femto-meter, the Coulomb potential energy is high enough that the electron, so bound, is necessarily relativistic.

For many decades, the question of the existence of electron deep levels or EDOs for the hydrogen atom has led to a number of works and debates. The issue was raised early in the solutions to the Klein–Gordon and Dirac equations, which became the basis of modern quantum mechanics. Therefore, it could have been given a high degree of credence as the field developed to become the mainstream of modern physics. However, without experimental evidence to support the unusual claims, this issue could not be resolved and the deep-orbit solutions are still considered to be anomalous. With the advent of low-energy-nuclear reactions, LENR, such evidence (albeit indirect) may now be available. What are these orbits and why are they suddenly more important now?

- EDOs, predicted in the anomalous solutions of relativistic quantum equations, have mean radii of their orbitals of order femto-meter. This is five orders of magnitude smaller than the known atomic orbitals.
- So, hydrogen atoms (including deuterium) with an electron in a deep orbit (femto-atoms) can facilitate processes of LENR inside condensed matter. This occurs by ready penetration of atomic electron clouds and nuclear Coulomb barriers, by the avoidance of nuclear fragmentation in $D-D \Rightarrow {}^4\text{He}$ fusion reactions, and by a means of increasing the rate of energy transfer between an excited nucleus and the surrounding lattice
- Moreover, femto-atoms can create femto-molecules and both can combine with lattice nuclei for transmutation without the normal resultant energetic radiations. This is not possible by other mechanisms.
- Mathematical arguments against the anomalous solutions of the relativistic equations have dominated the discussion of this issue for over 50 years. However, by acceptance of the physical reality of a non-singular central potential within a nuclear region, these objections no longer pertain.
- Numerical methods, available now with modern computers, readily allow prediction of properties and features of the EDOs from the exact equations that are not possible with the approximations made to keep the relativistic equations in the form of analytic functions.

Possibly the first application for the deep-electron orbits was in an early explanation of the nature of the neutron as a proton with a tightly bound electron. This particular concept was rejected nearly a century ago on theoretical physics grounds for several reasons [1]. This rejection would have been much more difficult to accept had the charge density distribution of the neutron that is available today been known at the time [2]. The negative outer edge, presently attributed to a negative pion cloud, certainly looks like a deep-orbiting electron.

Since the late 1950s, whenever the deep-orbit solution was rediscovered (every decade), it was immediately rejected based on mathematical, rather than on physical, reasons. Therefore, because the issue was never resolved and the importance of these unobserved orbits was so questionable, the difficult (perhaps impossible at the time) experiments to verify their existence were never even attempted and the issue never became general knowledge in the profession. Decades later, when experimental evidence for halo nuclei was obtained, rather than use the known, but largely forgotten, deep-orbit solutions that would introduce the beginning of a whole new nuclear chemistry and physics, physicists just stretched the strong nuclear potential beyond all expectations to explain the phenomenon.

With the advent of LENR phenomena and subsequent research, recognition that electron proximity between the hydrogen nuclei was necessary to overcome the Coulomb barrier again brought the deep-orbit solutions to the relativistic quantum-mechanical equations into focus [3,4]. However, the concept was unknown within the field and therefore almost ignored. By 2005, it was not even possible to publish papers in favor of the concept. (At that time, it was still possible to get a paper on the subject into the arXiv, [5].) On the other hand, papers showing that such deep orbits

were mathematically forbidden could still be published in physics journals. The present authors have spent the last year proving, in several papers [6–8], that the singular Coulomb potential ($V = k/r = -\infty$ at $r = 0$) used to reject the deep-orbit solution, can be replaced by a more realistic one (in several versions) and can lead to a valid, non-singular solution 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 e.g., [9]). 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 ^4He -fragmentation products, not to the observed atomic ^4He and heat of CF.” This problem is perhaps best addressed by the means and consequences of electron decay to the deep orbits [10,11].

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 [12]. 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 [13]. 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 [14,15]. 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 most-often-challenged 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? While there are several reasons, a straight-forward reason involves the lack of overlap of all atomic orbitals, except for the $l = 0$, s-orbits, with the deep-electron orbits. The normal electro-magnetic transition (via photons) between two $l = 0$ levels is highly forbidden. If the deep levels are unable to be populated in the natural environment and in the normal manner, then how are we to get electrons into these levels? This latter question has been addressed in part by [16–18].

Since the deep-orbit model can explain all of the observed CF results that we have addressed and is based on the fundamental equations of relativistic quantum mechanics, it should be readily accepted. 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.

2. Arguments against the EDO States and Possible Solutions

The most known arguments against the EDO states, while assuming a singular $1/r$ Coulomb potential, have been already exposed in [6] and in a more developed way in [7], as well as the possible solutions to resolve these questions. They concern only the radial solutions of the quantum equations. We quickly recall these arguments and some counter-arguments

2.1. The wavefunction has a singular point at the origin

For the solutions called anomalous, the radial function $|R(r)| \rightarrow \infty$ when $r \rightarrow 0$ and the wavefunction $\psi(r, \theta, \varphi)$ does not obey a boundary condition. In fact, this problem comes from the expression of the Coulomb potential in $1/r$. So, 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. Also, one can argue 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 EDO state. We indicate such solutions in Section 2.2.

We can add that, in the case of heavy nuclei, the accepted regular solutions of the relativistic Schrödinger equation also have a singular point at the origin, because the square of the coupling parameter $(Z\alpha)^2$ is not “small”; e.g. for atomic Cs, it is equal to ~ 0.16 , that gives $s \sim -0.2$ for $l = 0$ (for the parameter s , see Section 3.1.1).

2.2. The wavefunction is not square integrable

It is a serious problem, because in this case the wavefunction cannot be normalized in the entire space. As in Section 2.1., it results essentially from the behavior of the wavefunction ψ at the origin and not for $r \rightarrow +\infty$. Indeed, to define the norm of a wavefunction $\psi(r, \theta, \varphi)$ given in spherical coordinates, one has to compute $\int |\psi|^2 \sin \theta r^2 d\theta d\varphi dr = \int |Y(\theta, \varphi)|^2 \sin \theta d\theta d\varphi (\int |R(r)|^2 r^2 dr)$, where $Y(\theta, \varphi)$ are the so-called spherical harmonics, depending on quantum numbers l and m not indicated here. One knows the left integral is finite, while the right one depends on the behavior of $|R(r)|^2 r^2$ at the origin.

Here we can cite the work of Naudts [5], where an EDO state for hydrogen atom is found by using a Klein–Gordon equation, starting from a time-dependent *relativistic Schrödinger equation*. Because of chosen conditions on the parameters of the equation, the obtained solution is square integrable, thus normalizable. We have particularly developed explanations on this interesting result in [7], where the electron binding energy (BE) is very high in absolute value, with $|\text{BE}| \sim 507$ keV. We note the author only looks for solutions corresponding to spherically symmetric states, i.e. with angular quantum number (usually noted l) equal to 0.

Other works exist on singular states of the hydrogen atom, as e.g. in [19], where the author considers a compressed atom in a confinement potential described by a finite potential step at some given radius R_w taken at ~ 2.5 Å. A singular solution with deep orbits is obtained from a non-relativistic Schrödinger equation, by considering only the case $l = 0$, while using specific ansatz and approximation methods. But, because of the method used, the binding energy is not computed; neither is the mean radius. In fact, we think these levels could correspond to what we call pseudo-regular solutions [7].

Finally, we note most works on EDOs show that it is not possible to obtain square-integrable EDO solutions by means of the Dirac equations if keeping a Coulomb potential that is singular at the origin.

2.3. The orthogonality criterion cannot be satisfied

This mathematical condition, defined in a rather subtle way, corresponds to the fact the Hamiltonian, representing the total energy, must be a Hermitian operator, in order for its eigenvalues to be real, since they represent energy values of solutions. So, eigenfunctions corresponding to distinct values have to be orthogonal.

We can find in [20] the author 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 , and looks for conditions to satisfy known orthogonality criterion for the equation solutions. In particular the author eliminates the EDO solutions. Nevertheless, one can find in works on self-adjoint extension of operators for potentials with a singularity, e.g. in [21], a mathematical proof that singular solutions of the Klein–Gordon equation satisfy orthogonality for at least an angular momentum $l = 0$. However, no positive result can be proved for the EDO solutions of the Dirac equations.

2.4. The strength of the binding seems to increase when the coupling strength decreases

In [22], the author imagines variations of the coupling constant α and observes consequences on eigenfunctions of a Klein–Gordon equation and of a 2-D Dirac equation. Doing this, he points to a very strange phenomenon concerning

the algebraic expressions of the EDO solutions: when α decreases and tends towards 0, the binding energy of the electron increases in absolute value.

We think this result is obtained in the context of an ill-defined system and is done so, uniquely, on a pure mathematical basis. Indeed, the coupling constant α can be expressed by $\alpha = e/c\hbar$. So, from a physical point of view, we can see 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 binding energy).

2.5. Conclusion

As a quick conclusion of this section, we observed the following facts:

- The three first arguments against EDO automatically disappear if we consider the nucleus not to be a point, i.e. the Coulomb potential is corrected in order to have finite value inside the nucleus.
- Such a corrected Coulomb potential without singular point at the origin is necessary to accept EDO solutions of Dirac equation. Moreover, considering a nucleus with finite dimension has real physical meaning, especially if we look for deep orbit solutions, for which the mean radius is close to nuclear dimensions.

3. The Deep Orbits obtained as Solutions of Relativistic Equations

First, we quickly recall a specific work [3] on deep orbits, named Dirac Deep Levels (DDLs), as solutions of the relativistic Schrödinger and of the Dirac equations, which presented the most complete solution until recently. These solutions include an infinite family of DDL solutions for hydrogen-like atoms. Moreover, as these solutions were obtained by full analytic methods, the algebraic expressions of the energy levels point out an important fact: Special Relativity is essential to actually obtain deep orbits with high binding energy (in absolute value). This point is developed in Section 4. Next, we recall a second work [4] of the same authors, on solutions of Dirac equation for hydrogen-like atoms with a corrected potential near the nucleus. Then we report the results of a recent and complete analysis of this second work, with further developments and open questions. This analysis was required because of some criticism about the method used.

3.1. First results of Maly and Va'vra on "DDLs"

3.1.1. EDO obtained by using the relativistic Schrödinger equation

Maly and Va'vra consider the radial equation in the form given in ([23], 51.15):

$$\frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{dR}{d\rho} \right) + \left[\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1) - Z\alpha^2}{\rho^2} \right] R = 0. \quad (1)$$

They introduce an ansatz $R(\rho) = \rho^s e^{-\frac{\rho}{2}} L(\rho)$ in the radial equation, where $L(\rho)$ is a series of powers of ρ , s is a real parameter, and ρ is a real numerical parameter, without physical dimension but proportional to the radius r . Then, one can show that the eigenvalue energy E of the Hamiltonian is defined by the following expression, which is in fact the Sommerfeld relation:

$$E = mc^2 \left[1 + \left(\frac{(Z\alpha)^2}{\lambda^2} \right) \right]^{-1/2}, \quad (2)$$

where we recognize parameters λ and α of the prior equation. They are without dimension, but we have to note that α ($\sim 1/137$) is the coupling constant; for the hydrogen atom, we have $Z = 1$, that we consider hereafter.

Two conditions must be satisfied for obtaining convergence of the series $L(\rho): s(s+1) + \alpha^2 - l(l+1) = 0$, where l is the angular momentum quantum number, and $\lambda = n' + s + 1$, where n' is an integer number ≥ 0 . The first condition, a quadratic equation, has two roots: $s = -1/2 \pm [(l + 1/2)^2 - \alpha^2]^{1/2}$.

The usual regular solution for electronic energy levels is obtained by taking a positive sign in the expression for the root s , while a negative sign yields the so-called anomalous solution, giving the following expression for the energy levels:

$$E = mc^2 \left[1 + \frac{\alpha^2}{\left(n' + \frac{1}{2} - \left[(l + \frac{1}{2})^2 - \alpha^2 \right]^{1/2} \right)} \right]^{-1/2}, \quad (3)$$

where n' is the radial quantum number and l is the angular momentum quantum number.

The values represented by E are the total energy of the electronic orbitals. The corresponding binding energies BE are defined as $BE = E - mc^2$, which values have the usual negative sign.

In previous works, we showed that all energy values given by the expression of E do not correspond to deep orbits, but only the ones satisfying the relation $n' = l$, i.e. *equality between the radial quantum number and the angular quantum number*. Indeed, this condition allows one to drastically reduce the expression for λ :

From $\lambda = n' + s + 1$, $s = -\frac{1}{2} - [(l + \frac{1}{2})^2 - \alpha^2]^{1/2}$ and $n' = l$, we can deduce $\lambda \sim \alpha^2/(2l+1)$, as $\alpha \ll 1$.

Next, by carrying this into the expression of E , one can deduce $E \sim mc^2 \alpha / (2l+1)$. So, for all values of l , including the case $l = 0$, we have $E \ll mc^2$. Under these conditions, the binding energy $|BE|$ is very high and that means the orbit is very deep. There is an infinite family of these very deep energy levels with $|BE| > 507$ keV. Moreover, when the condition $n' = l$ is satisfied, we can note the following fact: if l (and thus also n') *increases*, then E decreases, which implies $|BE|$ *increases*.

So, *when the radial number increases, the electron is more strongly bound to the nucleus*, which is the opposite behavior of the atomic orbitals. As noted in Section 5.1, the coupling constant α exists in only the relativistic equations.

3.1.2. EDO obtained by using the Dirac equation

Maly and Va'vra refer to and use the method developed in [23], by starting with the system of radial equations obtained after separating the variables in spherical coordinates. We recall the Dirac equation, essentially relativistic since built from the relativistic expression of the total energy, has the following form in a central Coulomb potential:

$$(i\hbar\partial_t + i\hbar c \alpha \cdot \nabla - \beta mc^2 - V) \Psi(t, \mathbf{x})$$

where α and β represent the Dirac matrices, and α is in fact a 3-vector of 4×4 matrices built from the Pauli matrices. Here, V is the Coulomb potential, defined by $-e^2/r$.

During the solution process of the system of radial equations by using an ansatz, a condition on a parameter s occurs as an exponent. This condition in the ansatz, like the one appearing in the Schrödinger equation, as seen above, is the following: $s = \pm (k^2 - \alpha^2)^{1/2}$, where the scalar α again represents the coupling constant (do not confuse alpha with the Dirac matrices representation above). Also, as in Section 3.2.1, if taking the positive sign in the expression of s , one has the usual “regular” solutions for energy levels, then with the negative sign, one has the so-called “anomalous” solutions.

The expression obtained for the energy levels is the following:

$$E = mc^2 \left[1 + \frac{\alpha^2}{(n' + s)^2} \right]^{-1/2}. \quad (4)$$

We note this expression again has a form equivalent to the Sommerfeld relation, but where the parameter s has an expression slightly different from the one in Section 3.1.1. It contains the specific Dirac angular quantum number k instead of the usual orbital quantum number l .

If we consider the anomalous solutions, by choosing the negative sign s in the expression of E , this one reads:

$$E = mc^2 \left[1 + \frac{\alpha^2}{\left(n' - \sqrt{(k^2 - \alpha^2)} \right)^2} \right]^{-1/2}. \quad (5)$$

In this expression, n' is again the radial number, while k is the Dirac angular number which can take any integer value $\neq 0$. But hereafter, as k is involved everywhere in absolute value, we suppose $k > 0$. As in the case of the relativistic Schrödinger equation, all solutions do not correspond to deep orbits, but only the ones satisfying the relation $n' = k$, i.e. *equality between the radial quantum number and the Dirac angular quantum number*. Indeed, we can see that if $n' = k$, the sub-expression D of the total energy E , $D = n' - (k^2 - \alpha^2)^{1/2}$ becomes $D = k - (k^2 - \alpha^2)^{1/2}$, which is very small since $D \sim \alpha^2/2k$, and $E \sim mc^2\alpha/2k$. Then $|\text{BE}| \sim mc^2(1 - \alpha/2k)$ and $|\text{BE}|$ is close to the rest mass energy of the electron, 511 keV. Note that since k cannot be 0, then neither can n' .

From the expression of $|\text{BE}|$, we can deduce a result similar to the binding energies of the EDOs solutions of the relativistic Schrödinger equation. Under the condition $n' = k$ (necessary condition for EDOs), *when k increases, the absolute value $|\text{BE}|$ of the binding energy increases*. This means that, as the angular momentum k increases, *the electron is more strongly bound to the nucleus*. So, a natural question arose: what about the mean radius? Or more precisely, how does the mean value of the orbit radius progress as n' increases and tends to infinity? One could guess a partial answer to this question, while reading between the lines of the second work of Maly and Va'vra, which we recall in Section 3.2.

3.2. Deep orbits obtained as solutions of the Dirac equation with a corrected potential near the nucleus

In their second work [4], the authors determine the wavefunctions of EDOs, the so-called DDLs, for hydrogen-like atom solutions of the Dirac equation. They considered the nucleus not to be point-like, and thus the potential inside the nucleus is finite at the origin $r = 0$.

This requires one to carry out the following things:

- To choose a radius R_0 , the so-called matching radius, delimiting two spatial domains: an outside one, where the potential is correctly expressed by the usual Coulomb potential, an inside, where the potential cannot be expressed by the Coulomb potential and which no longer has a singular point at $r = 0$. Of course, this choice may seem arbitrary, but it takes physical meaning if one chooses a value R_0 close to the charge radius R_c of the nucleus. For example, for hydrogen H atom, the nucleus is reduced to one proton and this one has $R_c \sim 0.875$ F from CODATA [24]. So one can reasonably choose $1 \text{ F} < R_0 < 1.3 \text{ F}$.
- To choose a suitable expression for the inside potential. It is again an arbitrary point, but we observed (see further in Section 4.2.2) that this choice has weak influence on the numerical results that interest us, especially the value of mean radius as function of k .

- To satisfy continuity conditions at the matching radius R_0 for connecting the inside and outside potentials.
- Solve the system of radial equations for the outside potential, i.e. Coulomb potential, that gives the outside solution composed of two components: functions f_o and g_o .
- Solve the system for the chosen inside potential, that gives the inside solution composed of two components: functions f_i and g_i .
- To satisfy continuity conditions while connecting the respective components of inside and outside solutions.

In their work, the authors made the following choices and processes:

- For the matching radius, the value is not explicitly given in their paper, but from a figure, it seems $R_0 \sim 1.2 F$, but perhaps slightly smaller than this value.
- The chosen inside potential $V(r)$ has the following expression:

$$V(r) = - \left[\frac{3}{2} - \frac{1}{2} \left(\frac{r^2}{R_0^2} \right) \right] \frac{Ze^2}{R_0} + \beta_0. \quad (6)$$

- One can be surprised by the presence of the additive constant β_0 ; if it is not null, the continuity condition is not satisfied by the inside and outside potentials. Nevertheless, potential is relative and we will see further a possible usefulness of this constant. For the time being, we shall consider it is null.
- For finding the outside solutions f_o and g_o , they use the computation method of [25], a completely analytic method, where both components of the radial wavefunction, respectively, include functions F_1 and G_1 , expressed by means of confluent hyper-geometrical series.
- For the inside solutions, they choose an ansatz with two components, having the following form:

$$g_i = Ar^{S_i-1} G_2(r), \quad (7a)$$

$$f_i = iBr^{S_i-1} F_2(r). \quad (7b)$$

Where $G_2(r)$ and $F_2(r)$ are power series. However, one may consider approximations by polynomials, by taking into account the following facts:

- f_i and g_i must be defined for $r < R_0$.
- For $r < R_0$, very small, the power terms vanish when the degree increases.

The classical method used, after inserting the ansatz into the equations, allows one to determine the exponent s_i and the polynomial coefficients in order to obtain the solutions.

Nevertheless, it seems the cited paper was incomplete and useful information was in another paper of the same authors, referenced as “to be published” but never published. Indeed, the chosen ansatz does not allow one to connect both respective components of inside and outside solution, while respecting continuity conditions. A complete analysis of this problem, and the way we resolve it, is developed in [8]. Here, we simply recall the problem was resolved by taking a more complex ansatz including an additional real parameter λ necessary to connect in a suitable manner the inside and outside functions. In our ansatz, the series/polynomials have the following form:

$$G_2(r) = a_1(\lambda r) + a_2(\lambda r)^2 + a_3(\lambda r)^3 + \dots \quad \text{and} \quad F_2(r) = b_1(\lambda r) + b_2(r)^2 + b_3(\lambda r)^3 + \dots \quad (8)$$

The matching process leads to solving a system of two linear equations with two unknown variables, λ , involved in the inside solutions, and a multiplicative coefficient involved in the outside solutions; we showed the system always has solutions for any value of k , which determines energy levels. Moreover, we verified that the orthogonality criterion and boundary conditions are satisfied by each “global solution” formed by the respective outside and the inside solutions.

4. Results obtained by Computations of the DDL Wavefunctions for Modified Potentials, further Developments and Discussion

4.1. Computation process for orbit mean radii

The value of the mean radius is an essential parameter for the LENR, since the range of the strong nuclear force is on the order of femto-meters (fm or F) and quickly decreases at distances $> \sim 3-5 F$. The mean radius of its electron orbitals determines the “size” of the atom and the value of the repulsive radius of an atom. This radius can be estimated approximately [4] to be the value where the electron probability density drops to 1/10 of its peak value.

Summarily, the computation process for mean orbit radius *for a given value of k* includes the following steps:

- To determine both couples (f_o, g_o) and (f_i, g_i) of respective outside and inside solutions. At this step, the four functions $f_o, g_o, f_i,$ and g_i include parameters still to be determined
- To connect them in suitable manner and by satisfying the continuity conditions, in order to obtain a couple of global wavefunction solutions (F, G) . During this step, the unknown parameters included in the initial functions $f_o, g_o, f_i,$ and g_i are fixed. The functions thereby completely defined can be noted $F_o, G_o, F_i,$ and G_i .
- To compute the normalization constant N by using the following formula:

$$1/N = \int_0^{R_0} EL D_i dr + \int_{R_0}^{+\infty} EL D_o dr, \quad (9)$$

where $EL D_i$ represents the electron probability density corresponding to the couple of inside functions (F_i, G_i) :

$$EL D_i = 4\pi r^2 (|F_i|^2 + |G_i|^2) \quad (10)$$

and likewise $EL D_o$ for the outside functions

$$EL D_o = 4\pi r^2 (|F_o|^2 + |G_o|^2). \quad (11)$$

- Finally, to compute the mean radius $\langle r \rangle$ by using the following formula:

$$\langle r \rangle = N \left[\int_0^{R_0} r EL D_i dr + \int_{R_0}^{+\infty} r EL D_o dr \right]. \quad (12)$$

Now we have to note that, in principle, the numerical results of $\langle r \rangle$ should depend on the following preliminary choices:

- The choice of the matching radius R_0 : even if its value is reasonably chosen to fit physical data, such as the charge radius of the considered nucleus, it is rather fuzzy.
- The choice of the inside (nuclear) potential: apart from a common condition requiring it be finite at $r = 0$, there are multiple possibilities, each depending on modeling and approximations for the nuclear structure. Two of the most used examples are the following:
- A simple constant potential equal to the value of the Coulomb potential at the surface of the nucleus and corresponding to an uniformly charged empty spherical shell.

- The potential function defined by the expression written in the previous sub-section and corresponding to a uniformly charged solid sphere.

Nevertheless, one can consider more complex potentials, or intermediate forms of both previous ones.

- A more subtle choice, related to the precision of the inside functions, and depending on the approximation degree chosen for the polynomials of the ansatz, i.e. the power degrees of these polynomials.
- Of course, the choice of the considered hydrogen-like atom.

4.2. Numerical results

We carried out several series of computations for different choices listed in Section 4.1.

4.2.1. Results obtained from parameters near those of Maly and Va'vra

Here we first give the values of $\langle r \rangle$ computed for hydrogen atom H, while following approximately the choices of Maly and Va'vra:

- $R_0 = 1.2 F$.
- A nuclear potential defined by the expression given in Section 4.1 but assuming $\beta_0 = 0$. It approximates the proton by a uniformly charged solid sphere.
- The polynomials of our ansatz have degree 6, while the ones of M&V, for a simpler ansatz, have degree 5.

Under these conditions, we have the following values $\langle r \rangle$ for the mean orbit radii for different k values:

- $k = 1$, $\langle r \rangle \sim 6.62 F$,
- $k = 2$, $\langle r \rangle \sim 1.65 F$,
- $k = 3$, $\langle r \rangle \sim 1.39 F$,
- $k = 10$, $\langle r \rangle \sim 1.22 F$,
- $k = 20$, $\langle r \rangle \sim 1.20 F$.

The computed values are given with only three digits for high values of k , on account of uncertainties on the considered method.

We can note the following facts deduced from these computation:

- We obtain values of *the same size order* as that in [4], while we used *a method which is likely different*. 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 they give only this case for atomic H.
- The mean radius *decreases* when k *increases*, which is consistent with the fact that the binding energy in absolute value $|BE|$ *increases* when k increases, as expected in [6].
- After an abrupt fall between the value for $k = 1$ and the one for $k = 2$, the value of the radius *asymptotically tends to the value of the matching radius* 1.2 F. One can think there is an actual “accumulation sphere” at $r \sim R_0$, for the DDL orbits corresponding to $k \geq 20$, and these are indistinguishable.

In Fig. 1, we plot the near-nucleus normalized electron probability density functions (NEPD) for $k = 1, 2$, and 3.

4.2.2. Varying the parameters

Here we only report conclusions about results described in detail in [8].

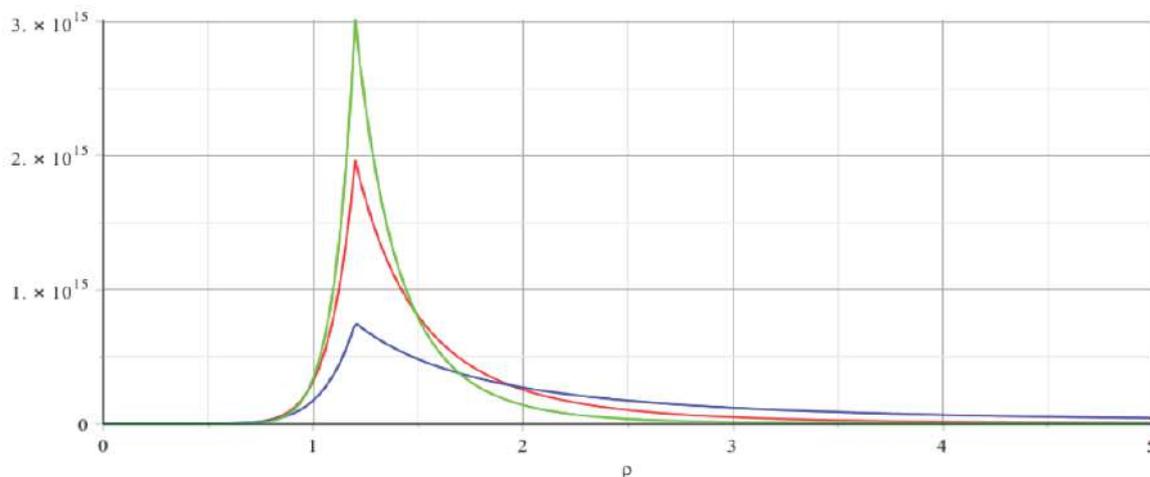


Figure 1. NEPD, for $k = 1$ (blue), $k = 2$ (red); $k = 3$ (green). The radius ρ is in F.

- With different values for R_0 , we obtain the *same kind of progression* when k increases, i.e. $\langle r \rangle$ *decreases* when k increases and $\langle r \rangle$ still *asymptotically tends to* R_0 .
- We also note a near-linear shift of the values of $\langle r \rangle$ in the same direction as the shift of R_0 . This effect is most important for the first values of k . For example, with $R_0 = 0.78$ F (not a reasonable value for atom H but only a style exercise) we obtain $\langle r \rangle \sim 4.6$ F for $k = 1$; and with $R_0 = 2.8$ F, which is reasonable for Li6 atom (it has charge radius $R_c \sim 2.59$ with $Z = 3$), we have $\langle r \rangle \sim 13.4$ F for $k = 1$.
- When taking polynomials of higher degree, we have still the same progression, but with slightly smaller values of $\langle r \rangle$ for the smallest values of k and then there is convergence.
- Surprisingly, a change of the nuclear potential has *almost no influence on the results*. Of course, we tested reasonable changes, i.e. such that the potential does not increase (in absolute value) for $r < R_0$. More precisely, we defined a parameterized potential, which can be fixed in intermediate forms between the potential previously tested and a constant potential for $r < R_0$, by the following expression:

$$V(r) = e^2(-\beta_1 + \beta_2 r^2), \quad \text{with } \beta_1 = (2 + \varepsilon)/2R_0 \text{ and } \beta_2 = \varepsilon/2R_0^3. \quad (13)$$

In fact, one can think the “inside” (i.e. nuclear) potential has only a very weak influence on the results, because the electron probability density inside the nucleus has a weak weight.

In conclusion:

- The values of the mean radius $\langle r \rangle$ are dependent on the angular number k .
- For any considered changes of the parameters, the *progression* of the values when k increases is *always the same*: the values of $\langle r \rangle$ decrease and tend to the value of the matching radius.
- The values of $\langle r \rangle$, globally, are nearly independent of the parameters except for the value of the matching radius R_0 . This seems logical from a physical point of view, when recognizing the charge radius of the nucleus. Nevertheless, the mathematical method introduces an intrinsic degree of arbitrariness in the choice of R_0 that cannot be eliminated.

4.3. Discussion on some criticisms about the considered method, and attempts to correct discrepancies

Here we consider two questions which arose about the method of corrected potential.

4.3.1. Question about the dependence of the inside solutions on the nuclear charge potential, and the coherence of the values of energies

On the one hand, we note a subtle criticism [26] about some lack of dependence of the solutions on the nuclear potential. By computation, we verified this lack of dependence (as indicated previously). On the other hand, if we compute, in an approximate manner, the value of binding energies BE corresponding to the computed values of the mean radius, we find some discrepancy.

For this question, we consider as test values, the values of mean radii $\langle r \rangle$ given at the beginning of the Section 4.2.1. for $k=1,2,3$, and 10. Effectively, if we compute binding energies corresponding to these radius values, while considering the simplified hypothesis where the electron orbits are quasi-circular, we obtain the following values of BE: -97 , -275 , -301 , and -320 keV corresponding to radius values 6.62, 1.65, 1.39, and 1.22 F, respectively.

These values have been computed by using the relativistic virial theorem [27,28], with the following relations:

$$PE = -\gamma mv^2 = -e^2/r, \quad KE = mc^2(\gamma - 1), \quad BE = KE + PE, \quad \text{Total energy } E = mc^2 + BE.$$

Of course, these calculations are carried out in a relativistic semi-classical way, but they give size orders having important shifts with respect to the starting values of BE for DDLs orbits, which are the following: -509 , -510 , -510.4 , and -510.8 keV with the same sequence. A possible reason is related to method of corrected potential. On the one hand, the inside functions are directly dependent on the nuclear potential $V(r)$, because this potential is inserted into the Dirac equation system to be solved. On the other hand, they involve DDL original energy values E (i.e. the ones indicated just above) inserted into the equation system, and so they indirectly depend on the Coulomb potential.

To correct this discrepancy, we use a method of iterative computation with convergence, which is precisely described in [8]. Summarily, at each computation cycle, one inserts energies, computed from previously computed radii, into the equations, until they reach a fixed point. We carry out this whole process for each $k = 1, 2, 3$, and 10 with following results:

- for $k = 2, 3$, and 10, the process reaches a fixed value at the first computation cycle, and we obtain the values of BE -275 , -301 , and -320 keV for radii 1.65, 1.39, and 1.22, respectively.
- for $k = 1$, as the successive values approximately behave as geometrical series; one can say there is convergence at radius value ~ 12 F, that would give BE ~ -56 keV.

In conclusion, we tend to think the actual DDLs for a modified potential will correspond to the results of this convergence process, which provides energy coherence and improved dependence of the inside functions on nuclear potential.

4.3.2. Question about a discontinuity of the derivative of solutions

A recent criticism was reported by a colleague, concerning the discontinuity of the derivative of the wave functions at the matching radius. Indeed, in the method for connecting the inside and outside functions at R_0 , for Dirac equation, one satisfies continuity only for the functions, but not for their derivatives. This seems to be a common practice, as the Dirac equation is a first-order differential equation. We can observe, in Fig. 1, that the electron probability functions also have discontinuities of the derivative at $\rho = 1.2$ F, as a consequence of the derivative discontinuity of the wavefunctions.

The criticism about this fact is the following: as the left-derivative and the right-derivative of the solutions are not equal at R_0 , one can deduce, *in reporting their values into the radial equations*, that the potential seems discontinuous at R_0 . This is equivalent to supposing an additional virtual potential ΔP at R_0 , creating a well or a barrier according the sign of ΔP . The author of this criticism claimed that the discontinuity and the virtual potential ΔP are needed for the existence of EDO.

One may ask why this happens, because if the inside and outside functions are solutions of the equations, the continuity of the derivatives should be automatically satisfied. Nevertheless, we must not forget that the inside solutions are obtained by polynomial approximations, which are less and less good when r increases and tends to R_0 . So the discontinuity, as well as the ghost potential, is actually a simple artifact due to technical imperfections of the method of corrected potential:

- There are not enough free parameters in the inside/outside solutions to satisfy *in the same time* (needed since the components f and g are coupled in the radial equation system) the continuity of both components f , g and the continuity of their derivative. The used ansatz (Section 3.2) allows us to satisfy only two equations, but not four equations required for continuity and derivatives.
- The polynomials approximations do not allow us to obtain the continuity of the derivatives at R_0 .

We can say the discontinuity of the wavefunctions has no relation with the existence of EDOs, since it was obtained as solutions of the Dirac equation with pure Coulomb potential. Wavefunctions with modified finite potential are needed only to satisfy mathematical properties (see Section 2) and to compute the mean radii $\langle r \rangle$ of orbits in a more realistic context (i.e., where the nucleus has dimension and the potential is finite). Nevertheless, we wanted to look for possible ways to study/correct this imperfection, while observing in all our computations of normalization constants and $\langle r \rangle$ (see Section 4.3.1) that the components of g , both the inside function g_i and the outside one g_o , dominate. This dominance of g over f can even reach several orders of magnitude for the outside functions when k increases.

So, to compute the mean radius $\langle r \rangle$ with the only largest component yields results close to the results with both components. Then we carried out numerous computations in various ways: e.g. to use the additive parameter β_0 (indicated in Section 3.2) as an additive potential to balance the virtual potential ΔP for the largest component, or to satisfy continuity and derivative continuity for this component. These computations always give results close to the ones indicated in the previous section.

As an example, in Fig. 2, we plotted a zoom of the large component of the wavefunction, satisfying both continuity and derivative continuity, with $k = 2$. For this one, we obtained 1.36 F instead of 1.6 F for the original solution. Of

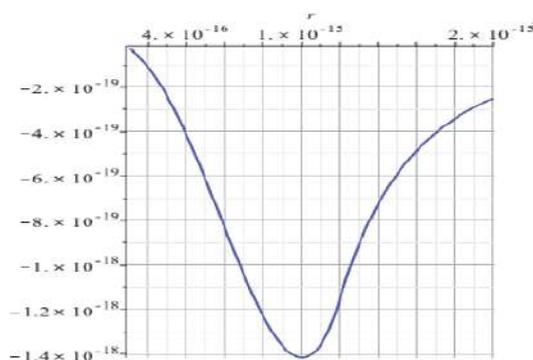


Figure 2. Large component g of the adjusted wavefunction for $k = 2$ and $R_0 = 1.2 F$.

course, it is an approximation since the computation was made only by using the component g . As a conclusion, we think it is not useful to look for a more complex method to resolve this question.

5. Why Special Relativity is needed to obtain EDOs with High Binding Energy

In previous works, we observe that non-relativistic equations give singular solutions, but these do not correspond to orbits with high binding energy (in absolute value). A physical reason is that an electron in a deep orbit is necessarily relativistic. So, it is more logical to use relativistic equations to find EDOs.

We also observed a pure mathematical reason which allows us to sort the EDO among the singular solutions of a relativistic equation, when we have analytic solutions at our disposal with energy levels E determined by an algebraic expression. Under these conditions, we can clearly see EDOs are obtained when a sub-expression, easily identifiable (see Section 3), can be drastically reduced. We saw such reductions are obtained by equating the radial number n' with the involved angular number (l or k). One can wonder if there is not a deeper reason behind this pure algebraic fact, in particular a reason having more physical meaning.

We have found such a deeper reason, first by comparing the relativistic version of the Schrödinger equation with its classical non-relativistic version and then by recognizing a relativistic correction to the potential, which is not taken into account for the usual atomic orbits because it is too weak at these energy levels. We have developed a complete analysis of this question in a paper [29] not yet published. Here we report only some essential elements and conclusion of this analysis.

5.1. Role and meaning of a relativistic parameter in the relativistic Schrödinger equation

The Dirac equation is essentially relativistic. On the other hand, as the Schrödinger equation has two versions, relativistic and non-relativistic, it is very easy to find parameters that make a difference. We can see that there is *one* parameter, which addresses our question and gives actual meaning to the involvement of relativity in EDOs.

We give both following versions of Schrödinger equations for the hydrogen atom, as extracted from [23]:

$$\frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{dR}{d\rho} \right) + \left[\frac{\lambda}{\rho} - \frac{1}{4} - \frac{l(l+1) - \alpha^2}{\rho^2} \right] R = 0, \quad (14)$$

$$\frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{dR}{d\rho} \right) + \left[\frac{\lambda'}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2} \right] R = 0. \quad (15)$$

The former is the relativistic one, already indicated in Section 3.1.1, while the latter is the non-relativistic one. They are expressed in terms of the dimensionless variable ρ for the radius, and R is the radial function, depending on ρ . We can observe that they are almost the same expression, except for the occurrence of an additional parameter, the coupling constant α , in the relativistic version. In [23] the equation contains the symbol γ instead of α , for a possible generalization at any atom with $\gamma = Z\alpha$. Of course, $\lambda \neq \lambda'$ and the transformation of the initial radius r into the dimensionless variable is not the same for both equations

5.2. The term α^2 is the source of EDO solutions

We already saw, in Section 3.1.1, that the energy levels are given by the following expression

$$E = mc^2(1 + \alpha^2/\lambda^2)^{-1/2}. \quad (16)$$

We also noted the EDO solutions are given by inserting $s = -\frac{1}{2} - [(l + \frac{1}{2})^{-1} \alpha^2]^{\frac{1}{2}}$ in the ansatz used for finding the solutions, since it provides a total energy of $E \sim mc^2 \alpha / (2l+1)$, when $n' = l$, and then a very high binding energy $|BE| = mc^2 [1 - \alpha / (2l + 1)]$, where the second term is $\ll 1$. The term α^2 occurring in the expression of E above directly comes from the one occurring in the relativistic equation.

It is not possible to set $n' = l$ in the case of the *non-relativistic equation*, where we recall that the singular solutions are obtained when taking $s = -(l+1)$. Here, the parameter λ' has to satisfy the condition $\lambda' = n' + s + 1$, for all types of solutions, which gives $\lambda' = n' - l$ for the singular ones. As the energy levels are given by $E = -mc^2 \alpha^2 / 2\lambda'^2$, one cannot reduce the expression for E by making $n' = l$, which would lead to $\lambda' = 0$ and thus to a singularity in the non-relativistic E .

5.3. What does the occurrence of α^2 mean?

The key to the answer is the fact the relativistic equation is built from the relativistic expression of total energy in free space $E^2 = c^2 \mathbf{p}^2 + m^2 c^4$, where \mathbf{p} is the momentum vector. Next one introduces an electromagnetic field in covariant form into the expression of E , and finally, since the nuclear Coulomb potential has spherical symmetry, one can write $(E - V)^2 = c^2 \mathbf{p}^2 + m^2 c^4$, where V is the Coulomb potential depending on the radius r . Afterwards, the expression $(E - V)^2 - m^2 c^4$, developed into $E^2 - m^2 c^4 - 2VE + V^2$, gives rise to several energy factors during the process of the Schrödinger building.

For example, the term λ/ρ occurring in the equation, and proportional to the Coulomb potential energy V , comes from $2VE$. However, it is the term $\gamma^2 l \rho^2$, *distinctive in the relativistic equation*, which interests us. It comes from and is proportional to V^2 . Moreover the parameter λ , used while building the dimensionless equation (14), is defined by $\lambda = 2E\alpha/\hbar c \varepsilon$ with $\varepsilon = [4(m^2 c^4 - E^2)/\hbar^2 c^2]^{1/2}$ one has $\lambda > 0$. By looking at this equation, one can observe the term $\alpha^2 l \rho^2$, greater than zero and proportional V^2 , is added to the term λ/ρ , which is greater than zero and proportional to V .

So, we find the real meaning of the occurrence of α^2 in Eq. (14) as cause of the existence of EDOs. It corresponds to a *dynamic relativistic correction to the Coulomb potential energy* V in the form of a term proportional to V^2 , which strengthens the static potential energy V .

Of course, the Dirac equation leads also to the same relativistic quadratic correction of the static potential V , but less directly visible than for the Klein-Gordon (or relativistic Schrödinger) equation. The general form of this correction (see e.g. [30,31]), but neglecting the centrifugal barrier paper, leads to the following effective “dynamic” potential:

$$V_{\text{eff}} = V(E/mc^2) - V^2/2mc^2. \quad (17)$$

Note that in the case of a relativistic electron, one can show $V_{\text{eff}} = \gamma V + V^2/2mc^2$, where γ denotes the well-known relativistic coefficient, i.e. $\gamma = (1 - v^2/c^2)^{-1/2}$.

Note also that, while looking at both expressions of V_{eff} given above, it is not clearly visible that one always has $|V_{\text{eff}}| > |V|$, i.e. a strengthening of the “normal” Coulomb potential. However, physically, since potential is an integral of the Coulomb force that increases as the electric-field lines of both the electron and central potential are relativistically compressed (strengthened), one would expect it to increase. Where the (effective) energy of the increased potential comes from and how it can exceed the static potential energy (normally) used to determine the invariant total system energy is another discussion.

Nevertheless, we showed in [29] that, at least in the case of quasi-circular orbits, we have the following result:

- One always has $|V_{\text{eff}}| > |V|$ and V_{eff} is attractive (a negative value),
- $|V_{\text{eff}}|$ quickly increases as a function of $|V|$, with a parabolic behavior in $|V|^2$ when $|V| \rightarrow +\infty$.

5.4. Computation of V_{eff} in the case of EDOs

Again with the quasi-circular orbits hypothesis, we computed the values of V_{eff} for the values of mean radii $\langle r \rangle$ given in Section 4.2.1. for EDOs orbits with $k = 1, 2, 3,$ and 10 and assuming $R_0 = 1.2 F$.

We have the following results for V_{eff} , where we indicate, at the same time, the values of $\langle r \rangle, V, \gamma, \Delta V = |V_{\text{eff}} - V|$, and the kinetic energy KE:

- $k = 1, \quad \langle r \rangle \sim 6.6 F, \quad \gamma \sim 1.2, \quad V \sim -218 \text{ keV}, \quad V_{\text{eff}} \sim -222 \text{ keV}, \quad \Delta V \sim 4 \text{ keV}, \quad \text{KE} \sim 120 \text{ keV},$
- $k = 2, \quad \langle r \rangle \sim 1.7 F, \quad \gamma \sim 2.2, \quad V \sim -873 \text{ keV}, \quad V_{\text{eff}} \sim -1.15 \text{ MeV}, \quad \Delta V \sim 277 \text{ keV}, \quad \text{KE} \sim 597 \text{ keV},$
- $k = 3, \quad \langle r \rangle \sim 1.4 F, \quad \gamma \sim 2.4, \quad V \sim -1.04 \text{ MeV}, \quad V_{\text{eff}} \sim -1.47 \text{ MeV}, \quad \Delta V \sim 430 \text{ keV}, \quad \text{KE} \sim 734 \text{ keV},$
- $k = 10, \quad \langle r \rangle \sim 1.2 F, \quad \gamma \sim 2.7, \quad V \sim -1.17 \text{ MeV}, \quad V_{\text{eff}} \sim -1.79 \text{ MeV}, \quad \Delta V \sim 620 \text{ keV}, \quad \text{KE} \sim 854 \text{ keV}.$

Of course, value uncertainties are great, therefore the numbers are rounded for clarity.

From the results above, we can see that, when k increases and as $\langle r \rangle$ decreases, γ and $|V_{\text{eff}}|$ increase because of relativistic effects and $|V|$ increases because the circularization of the orbits allows a lower average radius in the potential minimum. We also note that the ratio $\Delta V/\text{KE}$ increases with these changes because of the non-linear relativistic effects.

So, from a physical point of view, we can think the relativistic motion of the electron strengthens its effective potential energy in the Coulomb field, and even an increasing part of the kinetic energy seems “to act” on the strengthening ΔV of the potential energy, when the velocity of the electron increases. However, the effective potential used above does not include the centrifugal barrier that also increases with both k and γ .

6. Conclusion, Open Questions, Future Works

- At this point, we have reviewed the method of corrected nuclear potential applied to the deep-orbit solutions of Maly and Va’vra, we extended the results found by those authors and we found new results concerning the general properties of the deep orbits. Indeed, on the one hand, we have confirmed the order of values of mean radii $\langle r \rangle$ given by the authors. On the other hand, while varying the computational parameters, we observed that changes of values for $\langle r \rangle$ depend on few, other than the matching radius R_0 . Even if the choice of R_0 is a little arbitrary, this dependence is logical from a physical point of view when taking into account the charge radius of the nucleus (itself essentially related to the atomic number Z and the mass number A of the atom). We observed, in particular, a weak dependence of $\langle r \rangle$ on the inside functions, i.e. the solution inside the nucleus. In fact, the weight of the inside functions is about one half that of the outside functions.
- Concerning the general properties of the deep orbits, we had previously shown that the mean radii $\langle r \rangle$ decrease asymptotically to R_0 as the angular number k increases. This leads to the binding energy (in absolute value) increasing with k .
- Considering the weak dependence of results on our parametric variations, we can say the method is rather robust, a strength of this method of corrected potential.
- We also analyzed possible weaknesses of the method, identified in some criticism and in our own observations about the energy levels corresponding to the values of $\langle r \rangle$. The question of consistent energies for the values of $\langle r \rangle$ led us to a modified computation process assuming almost circular orbits. This gives the same values of $\langle r \rangle$ for $k > 1$, but almost doubles the radius for $k = 1$. The principal changes in the results concern new values of binding energy, which are significantly smaller (in absolute value) than those for the original EDOs. We think these values, from 275 keV (for $k = 2$) to 320 keV (for $k = 10$), with a limit $\sim 320 \text{ keV}$ as $k \rightarrow$ infinity, could be the actual values for EDOs. But this is still conjecture, because computations were made only with the simplified hypothesis of almost circular orbits. Anyway, we can note such modifications have

no implication for the existence of EDOs in the LENR process. Nevertheless, the lower binding energies of this computation greatly enhance the probability of populating the deep levels by near-field electromagnetic coupling of electrons in atomic orbitals with adjacent lattice nucleons and raising them to low-lying nuclear excited states.

- Another question is based on a discontinuity of the wavefunction derivatives at their matching point that leads to a virtual additive potential at R_0 . Nevertheless, while attempting to correct possible unwanted influence of this potential on the results, we observed by computation that there are no significant effects.
- Most importantly, we reveal the essential role of Special Relativity for the existence of EDOs with high binding energy due to the quadratic expression of the relativistic total energy. This leads to a dynamic correction to the original Coulomb potential and yields a noteworthy strengthening of the potential under some hypotheses. A more detailed analysis of the role of Special Relativity can be found in [29].
- Concerning open questions, the following is not yet resolved: the equality condition for radial number and angular number allows one to discriminate the true EDOs, characterized by strong binding energy, amongst the set of other singular solutions of equations, which have almost the same binding energies as the classical regular ones. In previous papers, we called these special non-EDO solutions, “pseudo-regular solutions.” In the same vein, we have not yet interpreted the meaning of these pseudo-regular solutions.
- Finally, a serious problem is still hanging over the existence of EDOs: do they respect the Heisenberg relation? Recent, but approximate, computations tend to answer yes to this question. Indeed, a first solution came from the spin-orbit interaction, which generates a very high attractive potential at the very small EDO radii. This potential exceeds that needed to provide the very high “Heisenberg kinetic energy” corresponding to electrons at these radii.
- To study the stability of EDOs, we still have to work more deeply on the properties of magnetic interactions and other possible effects near the nucleus, in order to evaluate the possible combinations of potential energies. In particular, the ones involved in the works of Vigier [32], Barut et al. [33] and Samsonenko et al. [34], and the correction to the Dirac operator due to the anomalous magnetic moment of the electron [35] might pertain.

Appendix added in Review

Up to now, we have worked on deep orbits as singular solutions of the Dirac equation, after analyzing, verifying and extending known works on this subject, such as those of Maly and Vav'ra [3,4].

Historically, the relativistic quantum mechanics for the electron became a field of quantitative science with the advent of the Dirac equations, which has subsequently been used for a very large number of applications. Indeed, many models for atoms, molecules and solids are based on many-electron generalizations of the Dirac equation. Nevertheless, we have now to take into account some known difficulties concerning this model of quantum physics. For example, where the generalization of the single-electron Schrödinger equation to the two-electron case immediately led to answers that compared well with experiment, the analogous generalization of the single-electron Dirac equation to the two-electron case led to the Brown–Ravenhall disease [36]. This problem (also referred as the continuum dissolution problem) is pointed out in virtually all works on many-electron questions. Summarily, it arises because solutions of Dirac equation form two continuums: the electron and positron ones; then, on double excitation of a pair of correlated electrons, one electron can end in the negative energy continuum (positrons), while the other lands in the positive energy continuum, the total system energy being retained. As a consequence, the number of such electron-positron states for an initial electron pair is infinite, and any energy level of the bound electron pair system is infinitely degenerate. This problem can be resolved by introducing special projection operators in the Hamiltonian to restrict it only to positive energy states, but of course one has no longer the classical “key in hand” analytic solution.

The Dirac equation includes other problems, such as e.g. the Klein paradox or also the fact, noted by Thaller [35],

that the Newton–Wigner operator (usually) taken as position observable leads to superluminal propagation.

Such problems lead us to introduce methods of quantum electrodynamics (QED) in our next works. Indeed, a critical feature in the construction of QED, which allowed a resolution for Brown–Ravenhall disease, was the complete elimination of the negative energy states for the description of electrons, and a corresponding complete elimination of the positive energy states for the description of positrons.

Moreover, QED became indispensable to continue our study, as it can take into account much subtle phenomena, such as, e.g. Lamb shift, which could be much more important near the nucleus than for atomic electrons.

Of course, as noted by Rusakova [37], the Brown–Ravenhall disease appears only in many-body cases. But the reviewer states our localized solutions of Dirac equations are in fact negative energy state solutions, after ending up analyzing such states in various ways. We think this could be a consequence of the fact the Dirac Hamiltonian is not bounded from below. As in QED, where the negative energy states are simply removed by construction from the available spectrum, the best way to resolve the question would be to try to look for deep orbits by using QED methods. One can even say that if there exists only one reason to introduce QED in our future work, it is this one.

Nevertheless, we have to recall [7] that the deep orbits, as singular solutions of Dirac equation, occur only when the angular number k and radial number n' are equal. This case, for $k = n'$, separates the positive- and negative-energy solutions. It falls on the positive-energy side. In fact there is a lot of other singular solutions: for $k > n'$, we explicitly get negative energy solutions, while for $k < n'$, we get solutions having almost the same (positive) energy levels as the regular ones (pseudo-regular solutions). As indicated in the conclusion above, we have not yet interpreted this situation, but one can think this profusion of weird solutions certainly introduces a big complication into the research of effective deep orbits.

Acknowledgement

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