

Research Article

Highly Relativistic Deep Electrons and the Dirac Equation

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Abstract

After analyzing, in the literature, deep orbit results of relativistic quantum equations, we studied them in a semi-classical way, by looking for a local minimum of total energy of an electron near the nucleus, while respecting the Heisenberg Uncertainty Relation (HUR). Now, while using new information thanks to semi-classical computations, we come back to deep electrons as solutions of the Dirac equation, to solve several important and subtle outstanding issues, such as the continuity of derivatives of wave functions, a spectral problem about the energy levels associated with the wave functions to compute, as well as essential relativistic and energy parameters of the solutions. We thus obtain a better completeness of the solutions. Finally, we give some approaches on the probability of the presence of Electron Deep Orbit (EDO) states in H atom.

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1. Introduction

Our works on the Electron Deep Orbits (EDOs) are motivated by the need to develop and complete a theoretical model to explain some of the outstanding questions about low-energy nuclear reaction (LENR) results. These results, such as the quasi-absence of high-energy radiation and ejection of particles, require an understanding of the nuclear processes involved [1,2] as well as the means of influencing them from a lattice. Moreover, a better understanding of EDOs and their interaction with nuclear fields will hopefully lead to a practical means of populating these deep levels in a nuclear region from which they can alter nuclear properties (e.g., transmutation and nuclear-decay processes [3]) and facilitate electron capture into the nucleus.

Over the last three years, we have analyzed results based on the use of relativistic quantum equations, because it was to be expected that an electron required to mediate fusion of two nuclei must maintain its high-probability of being between them and therefore must be relativistically or otherwise confined. That is why we particularly analyzed and extended [4] the results of [5] and validated [2] the need for relativity.

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In our more recent works, we took the question of the EDO from a different angle, by studying in a semi-classical way, the possibility of a local minimum of total energy for an electron in the vicinity of the nucleus. For this, we consider combinations of attractive and repulsive potentials [6], as well as the action of radiative corrections, such as the Lamb shift, while satisfying both the Heisenberg Uncertainty relation (HUR) [7,8] and the Virial theorem. Facing for the first time the thorny question of the HUR for electrons confined in deep orbits, we were able, not only to evaluate the coefficient γ of these highly relativistic electrons, but also to show that a strong relativistic correction to the Coulomb potential leads to an effective potential capable of confining such energetic electrons.

In the present work, being equipped with these new insights and methods, we come back to a important and subtle theoretical question encountered during initial EDO calculations with the Dirac equation, which showed a significant overlap of the electron wave function with the physical nucleus: Should the energy levels, usually obtained with the Dirac equation solved while considering a point-like nucleus, be modified and how? In fact, computation of the energy of a deep-orbit electron from its probability-density distribution, allows us to adjust its initial energy level by applying a fixed-point method. Moreover, we improve the semi-analytical solutions of the radial equations, to obtain wave functions having continuous derivatives on the femto-meter scale, including the surface delimiting the inside and outside of the nucleus. Doing this, we study how to preserve the initial coupling between the two components of Dirac solutions for EDOs. Finally, we give some approaches on the question of populating EDO states

2. Initial EDO Results, as Solutions of Dirac Equation for Atom H

2.1. The anomalous solutions of the Dirac equation

We had analyzed specific works of Maly and Vávra on deep orbits as solutions of the Dirac equation. These orbits were named by those authors Deep Dirac Levels (DDLs). They present the most complete solution and development available, including an infinite family of EDO solutions [9] for hydrogen-like atoms.

The Dirac equation for an electron in the central external Coulomb field of a nucleus, can take the following form:

$$(i\hbar\partial_t + i\hbar c \boldsymbol{\alpha} \cdot \boldsymbol{\nabla} - \beta mc^2 - V) \Psi(t, \mathbf{x}) = 0, \quad (1)$$

where $\boldsymbol{\alpha}$ and β represent the Dirac matrices, $\boldsymbol{\alpha}$ is a 3-vector of 4×4 matrices built from the well-known Pauli matrices, and V is the Coulomb potential, defined by $-e^2/r$. During the solution process with an ansatz, the following condition must be satisfied by a parameter occurring in the ansatz: $s = \pm(k^2 - \alpha^2)^{1/2}$. The scalar α represents the coupling constant (not to be confused with the vector of Dirac matrices $\boldsymbol{\alpha}$ occurring in the above Dirac equation). If taking the positive sign for s , one has the usual regular solutions for energy levels, whereas with the negative sign, one has the so-called anomalous solutions. The general expression obtained for the energy levels of atom H is the following:

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

So, while considering the anomalous solution, with negative s , the expression of E reads

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

where n' is the radial quantum number while k is the specific Dirac angular quantum number, which can take any integer value $\neq 0$. In fact, all solutions expressed by E do not correspond to deep orbits, but only those satisfying the relation $n' = |k|$ (note that k can be < 0). Indeed, we can see that if $|k| = n'$, the sub-expression D occurring at the

denominator of the expression E , $D = n' - (k^2 - \alpha^2)^{1/2}$, becomes $D = n' - (n'^2 - \alpha^2)^{1/2}$, which is very small since $D \sim \alpha^2/2n'$, and so $E \sim mc^2\alpha/2n'$. Then $|\text{BE}| \sim mc^2(1 - \alpha/2n')$ and $|\text{BE}|$ is close to the rest mass energy of the electron, 511 keV. Note, that since k cannot equal 0, then neither can n' .

Here, we summarize some features of the anomalous solutions of the Dirac equation [6]

- If $|k| > n'$, the solutions correspond to negative-energy states.
- If $|k| = n'$, these special solutions correspond to positive-energy states, and they are the only ones providing EDOs. Moreover, we can observe, in the energy tables in [9], the following property: the binding energy in absolute value, $|\text{BE}|$, increases when n' increases. This is a behavior opposite to that of the regular states. Note that one can also directly deduce this property from the algebraic expression of $|\text{BE}| \sim mc^2(1 - \alpha/2n')$.
- If $|k| < n'$, each solution corresponds to a positive energy state, but E is very close to the energy of a *regular level* corresponding to a value of the principal quantum number N taken equal to $n' - |k|$.

2.2. The deep orbits, as solutions of the Dirac equation with a corrected potential for a nucleus of finite size

In a second work [5], the authors determined the wave functions of EDOs for hydrogen-like atom solutions of the Dirac equation. But this time, they consider the nucleus not to be point-like, and thus the potential inside the nucleus is finite at the origin $r = 0$. We have seen, in the previous works on criticisms [10,11], that this allows eliminating the problems related to the singularity of the classical Coulomb potential in $1/r$.

To solve the Dirac equation, the authors use results from Fluegge [12]. As usual, the process includes separate angular and radial variables and leads to a system of coupled first order differential equations on both radial functions $f(r)$ and $g(r)$. In the method used by Fluegge, the equation system is transformed into a second order differential equation, a Kummer's equation, and the general solutions of this equation take the following form, with confluent hyper-geometrical series requiring suitable convergence conditions:

$$\begin{aligned} g &= \frac{1}{2}Cr^{s-1}e^{-r/a} \left\{ {}_1F_1\left(s+p, 2s+1; 2\frac{r}{a}\right) - \frac{s+p}{k+q} {}_1F_1\left(s+p+1, 2s+1; 2\frac{r}{a}\right) \right\}, \\ f &= \frac{-i}{2\mu}Cr^{s-1}e^{-r/a} \left\{ {}_1F_1\left(s+p, 2s+1; 2\frac{r}{a}\right) + \frac{s+p}{k+q} {}_1F_1\left(s+p+1, 2s+1; 2\frac{r}{a}\right) \right\}. \end{aligned} \quad (4)$$

Note: The parameters a and μ include the energy E defined by expression (2). For example, we have $\mu = [(mc^2 - E)/(mc^2 + E)]^{1/2}$; likewise, p and q are defined by means of μ , so they depend on E too.

To solve the equation with a nucleus of finite size $\neq 0$, the authors carry out the following steps:

- To choose a radius R , the so-called “matching radius”, delimiting two spatial domains: an outside one, where the potential is correctly expressed by the usual $1/r$ Coulomb potential, and an inside one, where the potential cannot be expressed by the Coulomb potential. Of course, this choice may seem arbitrary, but it takes physical meaning if one chooses a value R close to the charge radius R_c of the nucleus.
- To choose a suitable expression for the inside potential. It is again an arbitrary point, but we observed [4] this choice has weak influence on the numerical results that interested us, especially the value of mean radius as function of the radial number n' .
- To satisfy continuity conditions at the matching radius R for connecting the inside and outside potentials. The potential chosen by the authors is derived from the Smith–Johnson potential, corresponding to a uniformly distributed spherical charge, whose expression is the following:

$$V(r) = - \left[\frac{3}{2} - \frac{1}{2} \left(\frac{r^2}{R^2} \right) \right] \frac{Ze^2}{R}, \quad (5)$$

where $Z = 1$ for atom H, and e is the electron charge.

- To 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 . Here, the outside functions f_o and g_o are, respectively, the functions f and g expressed above while choosing $s < 0$, i.e. $s = -(k^2 - \alpha^2)^{1/2}$, to have anomalous solutions and by putting $|k| = n'$ to discriminate the special solutions corresponding to EDOs.

2.2.1. Ansatz used for finding the inside solutions and continuity conditions

The choice of ansatz is a very important element for finding f_i and g_i , solutions inside the nucleus, of the system of radial equations. Moreover, its expression is determinant to satisfy the continuity condition. A complete analysis of this question is given in [4].

In their paper [5], the authors put the ansatz in the following form:

$$g_i = Ar^{S_i-1}G_i(r),$$

$$f_i = iBr^{S_i-1}F_i(r),$$

where $G_i(r)$ and $F_i(r)$ are in principle power series, i.e.

$$G_i(r) = a_1r + a_2r^2 + a_3r^3 + \dots \quad \text{and} \quad F_i(r) = b_1r + b_2r^2 + b_3r^3 + \dots$$

But one may consider approximations of these series by polynomials by taking into account the following facts:

- f_i and g_i must be defined for $r < R$.
- For $r < R$, very small, the higher-power terms vanish as 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. This requires solving a couple of interdependent recurrent formulas for computing the coefficients of both power series $G_i(r)$ and $F_i(r)$. Nevertheless, it seems the information given in the paper is incomplete, or more precisely, the chosen ansatz is not complete and it does not contain enough free parameters to satisfy the continuity condition for both couples of functions (f_i, g_i) and (f_o, g_o) in R . In fact useful information was included in another paper by the same authors, referenced as to be published, but never published.

To resolve this problem, we looked for a more complex ansatz including an additional free real parameter λ , necessary to connect in a suitable manner the inside and outside functions, where the series/polynomials have the following form:

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

The continuity conditions $\{g_i(R) = g_o(R), f_i(R) = f_o(R)\}$ lead to a system of two algebraic equations. We showed in [4] that, for any degree n of the polynomials, the maximum power of λ in this system of equation remains constant and equals 2, and so this system provides suitable solutions.

2.2.2. Computing the orbital mean radii

Summarily, the computation process for mean orbit radius for a given value of n' 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 a suitable manner, e.g., by satisfying the continuity conditions, in order to obtain a couple of global wave function 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 denoted by F_o, G_o, F_i , and G_i
- To compute the normalization constant N by using the following formula:

$$1/N = \int_0^{R_0} \text{ElDi} \, dr + \int_{R_0}^{+\infty} \text{ElDo} \, dr,$$

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

$$\text{ElDi} = 4\pi r^2 (|F_i|^2 + |G_i|^2).$$

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

$$\langle r \rangle = N \left[\int_0^R r \, \text{ElDi} \, dr + \int_R^{+\infty} r \, \text{ElDo} \, dr \right].$$

2.2.3. Obtained results and discussion on imperfections

We give some examples of wave function solutions computed for the hydrogen atom H, while using the following choices

- $R = 1.2 \, \text{F}$,
- A nuclear potential defined by expression (4) given previously, where the proton is approximated by a uniformly charged solid sphere,
- The polynomials of our ansatz have degree 6.

In Fig. 1, we plot the *normalized electron probability density functions* (NEPD) for $n' = 1, 2$, and 3. The peak values for NEPD correspond to $r \sim R$.

Values of mean radius $\langle r \rangle$ and total energy E for $n' = 1, 2$, and 3. Note that in these computations, E is deduced from Eq. (3), which gives $E \sim mc^2 \alpha / 2n'$.

- $n' = 1, \langle r \rangle \sim 6.6 \, \text{F}, E \sim 1.86 \, \text{keV},$
- $n' = 2, \langle r \rangle \sim 1.7 \, \text{F}, E \sim 0.93 \, \text{keV},$
- $n' = 3, \langle r \rangle \sim 1.4 \, \text{F}, E \sim 0.62 \, \text{keV}.$

Now, we can make the following remark: to find out how to populate deep levels, an essential and concrete question about utility of EDOs for LENR, we need to know more information and to correct some imperfections. These are listed here in the form of three problems, in an order that has no significance of importance.

- Problem #1. The ansatz we had used does not allow us to have continuous derivatives at the connection radius R . This problem is more serious than it appears at first sight. The initial Dirac equation and the resulting system of two radial equations, after separating the variables, are 1st order equations. Nevertheless, the radial equations are not independent (see e.g. [13]) but interdependent, as both components f and g occur in each equation. In fact the system is equivalent to a differential equation of second order, and it is completely

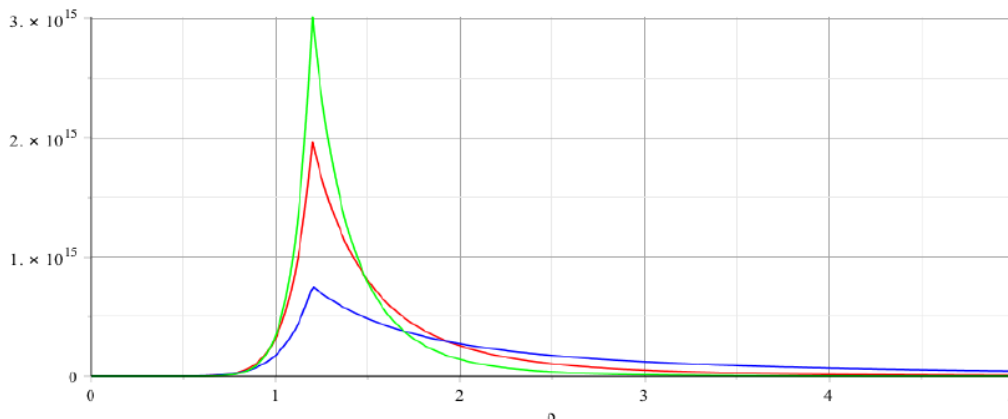


Figure 1. NEPD, for $n' = 1$ (blue), $n' = 2$ (red), $n' = 3$ (green), with $n' = |k|$. The radius ρ is in F.

solved by using effectively a second order equation, e.g. a Kummer's equation [14] or a Whittaker's [15] equation. Under these conditions, it is mathematically necessary for the global solution function to be not only continuous, but also to have a continuous derivative everywhere in the domain of real numbers. In [16], we have obtained this result for the large component, but it is an approximation, and it should be extended to both components to have better information on the wave functions.

- Problem #2. Expression (4), used to compute the wave function (in fact the part outside the nucleus), depends on an energy parameter E occurring in its parameters a, μ, p , and q . But the value of the energy E is the energy of solution for a point-like nucleus case. This is not really suitable in the case of the solution for a nucleus of finite size with a corrected potential.
- Problem #3. It is difficult to correctly evaluate the relativistic coefficient γ and the energy parameters, such as the kinetic energy, required for a better understanding of EDOs and possible interaction of deep-orbit electrons with nuclear fields.

Finally, it should be noted that there was a rather serious problem, in our early work on EDO solutions of the Dirac equation, about the HUR, apparently unsolved also in similar works existing in the literature: how can electrons confined in EDOs, very close to the nucleus, respect the HUR? This issue has been solved in an unexpected way, through the use of relativity, and a change in strategy towards HUR. Therefore, it is not indicated in the previous list and the solution, explained in detail in recent works [7], is briefly recalled in Section 3.

3. Semi-classical Computations/Simulations

To better know the energy parameters of EDOs and their possible existence, we made semi-classical studies [6–8] with many computations, by applying the following principles:

- We consider a radial potential energy PE built as a sum of inverse power terms, including the Coulomb potential, magnetic interactions, and possibly radiative corrections.
- We look for a local minimum of energy (LME) for an electron near the nucleus, while we consider its total energy TE including the potential energy PE. TE is specified below.
- But, most important for stable orbits, the HUR must be respected.

3.1. Special relativity and the HUR

3.1.1. Respecting the HUR

We decided to take HUR as a starting point, while considering an electron confined near the nucleus. We previously showed [2] that Special Relativity is necessary to have deep orbit solutions of quantum equations. Nevertheless, while starting from HUR [6,7], we find that the relativistic coefficient γ expected for EDOs had been greatly underestimated. In fact, electrons confined in deep orbits (EDO), with mean radius of order a few F, are highly relativistic (γ can be > 200). Here we summarily give some elements and results, specified in detail in the quoted references.

For an electron confined in a sphere of radius r , from momentum $|\mathbf{p}| \sim \hbar / r$ (to respect the HUR), and from its relativistic expression $p = \gamma mv$, we can deduce the following results:

$$\gamma = (1 - v^2/c^2)^{-1/2} \sim [1 + (\underline{\lambda}_c)^2/r^2]^{1/2} \quad (6)$$

where $\underline{\lambda}_c$ denotes the “reduced” Compton wavelength, i.e. $\underline{\lambda}_c = \hbar/mc$. For electrons, one has $\underline{\lambda}_c \sim 386$ F. For EDOs, as it seems that $r \ll \underline{\lambda}_c$, γ can be simplified into $\gamma \sim \underline{\lambda}_c/r$. We gave examples [8] showing expression (6) gives realistic and rather precise values.

3.1.2. Relativistic correction of the Coulomb potential energy and confinement of electron in deep orbit

Because of the high level of the relativistic coefficient γ , it is interesting to consider the effects of the relativistic correction to the static Coulomb potential, as indicated in [17,18], under the resulting form of an effective dynamical potential noted V_{eff} , and already considered in [2,16]. The general form (3) of V_{eff} comes from the development of relativistic quantum equations (Dirac, Klein–Gordon) with the expression of the relativistic energy of a particle in a central field for a Coulomb potential energy V :

$$V_{\text{eff}} = V(E/mc^2) - V^2/2mc^2. \quad (7)$$

On the other hand, by replacing E by an approximate value γmc^2 in (7), we obtain the following form (8) including the coefficient γ :

$$V_{\text{eff}} = \gamma V - V^2/2mc^2. \quad (8)$$

While putting the full expression (6) of γ into (8), we obtain V_{eff} as a function of r , where α is the coupling constant:

$$V_{\text{eff}} = -(\alpha c \hbar / r) ([1 + (\underline{\lambda}_c)^2/r^2]^{1/2} + \alpha \underline{\lambda}_c / 2r). \quad (9)$$

Finally, if r is of order a few F, one can obtain the following approximate form:

$$V_{\text{eff}} \sim \gamma V. \quad (10)$$

So, we have the two following results:

- (1) V_{eff} is always attractive
- (2) $|V_{\text{eff}}| \geq |V|$, i.e. V_{eff} is always a strengthening over the static Coulomb potential energy.

Moreover, and most importantly for the EDO's, we showed in previous works [7,8] that V_{eff} can easily confine an electron near the electron. Indeed, for r very small, the kinetic energy $\text{KE} = (\gamma - 1)mc^2$ has behavior in $1/r$, whereas V_{eff} has behavior in $1/r^2$. More precisely ([8], Fig. 1) we showed that for $r < 2.8$ F, one has $|V_{\text{eff}}| > \text{KE}$.

In fact, Relativity involvement, as defined by the HUR constraint on KE, is the solution for EDO confinement.

3.2. Semi-classical computations of EDOs

In order to find EDOs, we look for a Local Minimum of Energy (LME) of electron in a central potential PE, obtained by a balanced combination of electro-magnetic (EM) potentials near the nucleus. The total energy is equal to TE = E_H + PE, where E_H is defined by the following expression:

$$E_H = \sqrt{\frac{\hbar^2 c^2}{r^2} + m^2 c^4} \quad (11)$$

It is obtained from the relativistic expression of energy of a free electron, $(\mathbf{p}^2 c^2 + m^2 c^4)^{1/2}$, by putting $|\mathbf{p}| \sim \hbar/r$ for respecting the HUR. Note that $KE = E_H - mc^2$.

In previous work [7], we built a combination of EM potential energies, inspired by a study [6] of the Vigier–Barut model [19–24] and related works, then we took radiative corrections into account, i.e. essentially the Lamb shift (LS) [25–29], including two phenomena: electron Self-Energy (SE) and Vacuum Polarization (VP). In fact, the LS supplies a specific extra energy, corresponding to a *decrease of the binding energy*. So it has a global repulsive effect on the bound electron.

We made numerous computations of LME with variants on the combinations of EM potentials. Here, we give only a variant of example from [8], where the LS is expressed as a repulsive quasi-potential energy by means of extrapolations from known data tables on QED effects on orbital parameters. In fact, we put $V_{LS} = 0.623 \times 10^{-10} / \rho^3$ in J/F³. In Fig. 2, we plot an example curve of the binding energy BE = KE + PE = TE - mc^2 , where the LME corresponds to $\rho \sim 1.4$ F.

In this example, the main parameters of the electron at the LME (at $\rho \sim 1.4$ F) have the following values:

- $\gamma \sim 275$,
- BE ~ -509 keV,
- PE ~ -140.5 MeV,

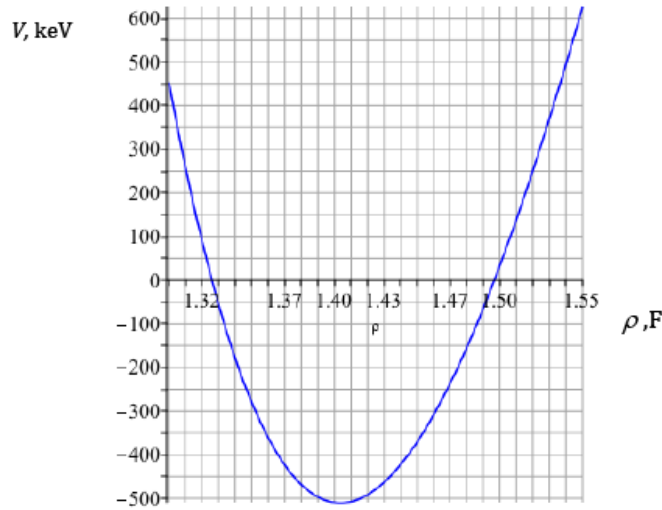


Figure 2. Plot of electron BE, for $1.3 \text{ F} < \rho < 1.55 \text{ F}$.

- $KE \sim 140 \text{ MeV}$.

3.3. Key information from semi-classical calculations

Semi-classical studies provided a lot of useful information for correcting the imperfections of the initial Dirac EDO's for finite nucleus case. Not only we can evaluate the relativistic coefficient γ , but also all the energy parameters. Moreover we found that the relativistic *Virial theorem* [30] *was respected by ultra-relativist EDOs*, in a very simple form and for various combinations of potentials. So, we can see that

- Electrons confined near the nucleus are ultra-relativistic.
- The relativistic Virial theorem is respected at the LME, in the following form: $KE/|PE| \sim \gamma/(\gamma + 1)$.

This allows us to deduce all the main parameters of the Dirac EDOs, computed at the mean radius of the probability density distribution, and to check their coherence: With a corresponding LME radius $\longrightarrow$ mean radius $\langle r \rangle$ of Dirac EDO solutions with finite nucleus, we can evaluate γ , TE, KE, and BE at $\langle r \rangle$. For example, one can show $TE \sim m_e c^2 / \gamma \sim m_e c^2 \langle r \rangle / \lambda_c$.

So, we can correctly adjust the energy levels of Dirac EDO's solution (see Problem #2), and know all the energy parameters (see Problem #3).

4. How to Apply the New Information Provided by Semi-Classical Computations, to Dirac EDOs?

4.1. A brief reminder of what the solution of a quantum equation for wave function consists of

Such a quantum equation generally has the following form: $H\psi = E\psi$. Summarily, we have two concomitant mathematical issues.

- (1) H is a “Hamiltonian”, representing the total energy of the considered system. It is generally a Hermitian operator including differential operators. For example, the momentum $\mathbf{p}$ is expressed by the expression $-i\hbar \frac{\partial}{\partial \mathbf{X}}$, including a vector of partial derivatives on spatial coordinates, $\frac{\partial}{\partial \mathbf{X}}$.
Note a Hamiltonian can be multidimensional (e.g. in the Dirac equation). *So, we have to solve a differential equation.*
- (2) We look for ψ , an unknown wave function, and for E , unknown eigenvalues, which are *energy values* associated with eigenvectors ψ *corresponding to wave function solutions*. These can be characterized by integers, quantum numbers, if the set of eigenvalues is a discrete set, *composing energy levels*.

So, we have *to solve a spectra problem* [31] for H atom: to find eigenvalues associated with solutions of the differential equation.

4.2. Solving the Dirac equation for hydrogen atom with finite nucleus

4.2.1. Solving the system of radial differential equations

After separation of the angular and radial variables, one ends up with a system of two radial equations.

As we consider a H atom with non-point-like nucleus of radius $\sim R$, we have to solve radial differential equations, where the radius belongs to two separate domains of the real numbers, associated with the inside and the outside of the nucleus respectively. And the central potentials are very different in these domains.

- (i) Outside the nucleus, the static potential energy corresponds to the classical Coulomb potential, and is expressed by means of the formula $V_O = -e^2/r$, where e is the charge of the electron (expressed in suitable units).

- (ii) Inside the nucleus, the potential energy V_I is expressed by the chosen formula (4), with $Z = 1$, equivalent to $V_I = -(e^2/2R)(3 - r^2/R^2)$.

So the whole potential energy is described by a *piecewise* expression:

$$\text{Pot}(r) = V_I \quad \text{if } 0 \leq r \leq R \quad \text{and} \quad = V_O \quad \text{if } r > R.$$

As a consequence, the differential equation $\text{Eq}(r)$, using $\text{Pot}(r)$, will have a piecewise form:

$$\text{Eq}(r, \text{Pot}(r)) = \text{Eq}_I(V_I) \quad \text{if } 0 \leq r \leq R \quad \text{and} \quad = \text{Eq}_O(V_O) \quad \text{if } r > R.$$

The software used for differential equations, Maple, can solve any differential equation on a limited domain. For the system of Dirac radial equations, we can observe the following:

- (1) First, the formal solutions are very different in the two domains. As complex expressions including very different special functions (defined by series), they are very difficult to unify.
- (2) A solution on the limited domain considered (here the domain outside the nucleus) is formally the same as on the whole domain of real numbers.

Note we apply this reasoning only on the limited domain outside the nucleus: for the very small domain inside the nucleus, it is sufficient to solve the differential equations approximated by polynomials.

From the point #2, we deduce *the general solution for point-like nucleus case*, i.e. the solution on the whole domain of real numbers, *can be used for the domain associated with the nucleus outside*. So, for this domain, we can use, in principle, the solution indicated in Section 2.2, i.e. expression (4) of the pairs of functions (f, g) . Nevertheless, as noted in Problem #2, Section 2.2.3, expression (4) used to compute the wave functions solutions of the radial equations, depends on an energy parameter E occurring in the expressions of several parameters, a, μ, p, q . But the only value of E that we know is the one given by formula (3), corresponding to the energy levels of Dirac solutions for point-like nucleus case. Of course this is not really suitable in the case of solution for a nucleus of finite size with a corrected potential. When applying the *general solution to limited domain* $r > R$, for solutions *outside the nucleus*, the eigenvalue E' associated with the wave functions (f_O, g_O) must be different from the energy E of general solutions for point-like nucleus. So, *we have to solve a spectral problem*.

To address this issue, we use a kind of perturbative method, in the form of iterative computation until we reach a fixed point. It is explained in Section 4.2.3.

4.2.2. Connecting inside and outside solutions (Problem #1)

Before the fixed-point process, we consider the question of connecting the couples of inside and outside solutions at the nucleus surface, with continuity of the total functions and their derivatives.

More precisely, the couples of inside (f_I, g_I) and outside (f_O, g_O) solutions have to be *connected* at the surface of the nucleus, under the following conditions (Problem #1, Section 2.2.3):

- (1) We must satisfy the *continuity* at $r = R$, i.e. $f_I(R) = f_O(R)$ and $g_I(R) = g_O(R)$.
- (2) We must satisfy the *continuity of respective derivatives*

$$f'_I|_R = f'_O|_R \quad \text{and} \quad g'_I|_R = g'_O|_R.$$

Here we indicate, in a rather brief and simplified way, the successive steps that allow us to satisfy these conditions.

The functions f_O and g_O determined by expression (4), include the same multiplicative constant C , because of the coupling of the radial equations: i.e. we have $f_O = C \text{Expf}$, $g_O = C \text{Expg}$, where Expf and Expg are the expressions deduced from the computation of (4) and represent two functions of the radius r .

- I As a first step, we decouple these two functions, while writing $f_O = C1 \text{Expf}$ and $g_O = C2 \text{Expg}$.
- II (a) While using an ansatz as in Section 2.2.1, we compute a polynomial P_f as an approximation of f_1 . So f_1 is expressed in powers of the radius r and includes the free parameter λ_f .
We compute also the derivative f_1' in r of f_1 ; f_1' also includes the free parameter λ_f .
(b) Then, we compute the derivative $f_{O'}$ in r of the function f_O . Of course, the function $f_{O'}$ includes the multiplicative parameter $C1$.
(c) Finally, we calculate $f_1(R)$, $f_O(R)$, $f_1'(R)$ and $f_{O'}'(R)$, where R is the “junction” radius between the inside and outside of the nucleus. Then we solve the system of equations $\{f_1(R) = f_O(R), f_1'(R) = f_{O'}'(R)\}$. The solution of this equation gives a result in the form $\{C1 = a, \lambda_f = b\}$, where a and b are two real numbers, and we replace $C1$ and λ_f by their values in the expressions for f_1 , f_O , f_1' , and $f_{O'}'$.
- III A similar process is applied to the second component, represented by the couple of functions (g_1, g_O) , which leads, after solving a system of equation at the junction radius R , to a result having the form $\{C2 = c, \lambda_g = d\}$, with two real numbers c and d .
- IV In order to restore the initial coupling of components f and g , we put $F_1 = cf_1$, $F_O = cf_O$ and similarly for their derivatives (just for checking the condition (ii) above).

For the g components, we multiply by a , i.e. $G_1 = ag_1$, $G_O = ag_O, \dots$

Finally, we denote, by $F = f_1 U f_O$, the total function obtained by connecting f_1 with f_O at $r = R$, and similarly $G = g_1 U g_O$.

4.2.3. Fixed point method for solving the spectral problem (Problem #2)

We indicate in very simplified form, the iterative process used. Starting point: for a given value of radial quantum number n' , expression (3) of energy for solution in the point-like nucleus case, gives a value noted E_0 .

- Step 0: we take E_0 to determine the total wave function $\Psi_0 = (F, G)$, as explained in the prior sub-section, and we compute the electron probability density. Then we deduce the average orbital radius r_0 and we can directly calculate the total energy E_1 of electron at r_0 , as explained in Section 4.3. Next we will go to Step 1, where a new value r_1 of orbital radius is computed.
- Step 1: Normally we have $E_1 \neq E_0$. Then, as in Step 0, E_1 determines a new wave function Ψ_1 and we compute the mean orbital radius r_1 from the new electron probability density distribution. From this, we calculate the new energy E_2 at the radius r_1
 - If $E_2 \sim E_1$ (up to three digits), we consider that we reached a fixed point.
 - If $E_2 \neq E_1$, we go to a Step 2 similar to Step 1.

In fact, many computations, for different values of the radial number n' and even by varying the “initial” value of energy E_0 , lead to the following observations:

- The mean radius corresponding to wave function Ψ varies very slowly as a function of the energy E injected in expression (4) to calculate Ψ .
- At Step 1, r_1 is already close to r_0 .
- We can stop the process at Step 1 to check that the fixed point is practically reached and, if so, take Ψ_1 as a wave function solution of the problem and E_1 as total energy of this solution.

4.2.4. EDO solutions of Dirac equation for H atom with finite nucleus

In Fig. 3, we plot the curves of normalized probability density corresponding to $n' = 1$ and $n' = 2$, while considering a junction radius $R = 1$ F, and for $0.4 \text{ F} < \rho < 3 \text{ F}$, where ρ denotes the radius in F.

We give the mean radius $\langle \rho \rangle$, and the values of the relativistic coefficient γ and the kinetic energy KE, which were not obtained with the initial results indicated in Section 2. Moreover, we compare the values for the total energy, denoted by TE, and the binding energy BE obtained with our new method, with those obtained in the initial solutions, corresponding to the point-like nucleus case (PLN), written in italic.

- $n' = 1$, $\langle \rho \rangle \sim 4.5 \text{ F}$, $\gamma \sim 84$,
KE $\sim 42.5 \text{ Mev}$, TE $\sim 6 \text{ kev}$ (1.8 kev, PLN), BE $\sim -505 \text{ kev}$ ($\sim -509 \text{ kev}$, PLN).
- $n' = 2$, $\langle \rho \rangle \sim 1.13 \text{ F}$, $\gamma \sim 405$,
KE $\sim 206 \text{ Mev}$, TE $\sim 1.5 \text{ kev}$ (1 kev, PLN), BE $\sim -509.5 \text{ kev}$ ($\sim -510 \text{ kev}$, PLN).

Moreover, one can verify the mean radius $\langle \rho \rangle$ and the total energy TE satisfy the following relationship: $\langle \rho \rangle \sim \lambda_c \text{ TE}/mc^2$, where λ_c is the reduced Compton wavelength ($\sim 386 \text{ F}$) and m is the electron mass.

5. Can EDO States be Populated?

5.1. Heisenberg barrier

Here is a first attempt to evaluate a possible population of EDO states by tunneling from the atomic-electron ground state, in the form of superposition of quantum states. To simplify the situation, we consider only two antagonistic interactions, one due to the attractive relativistic effective potential energy V_{eff} , and the other to the HUR, increasing the kinetic energy to prevent the containment of electron: we call it Heisenberg barrier ([8], p. 478).

These are not static fields, but *dynamic effects* associated with a possible increasing confinement of the electron.

- On one hand, we consider the kinetic energy $\text{KE} = (\gamma - 1)mc^2$.

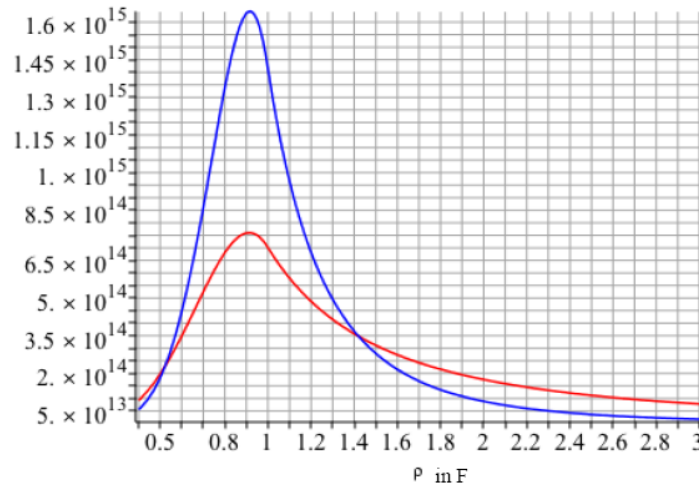


Figure 3. Plot of the normalized probability density, for $n' = 1$ (red) and $n' = 2$ (blue).

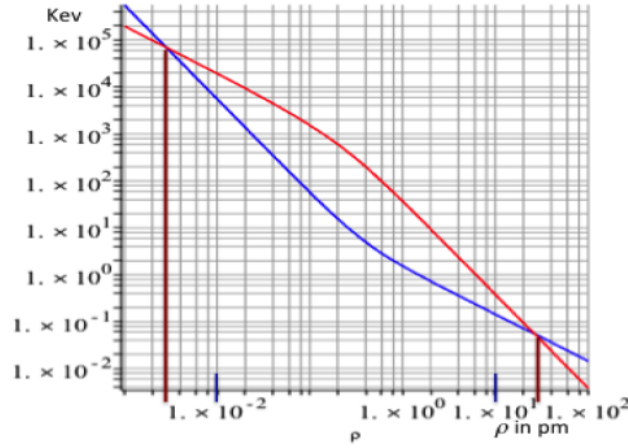


Figure 4. Loglogplot of KE and $|V_{\text{eff}}|$ for $1 F < \rho < 100$ pm.

- On the other hand, the relativistic effective potential energy $V_{\text{eff}} = \gamma V - V^2/2mc^2$, where the relativistic coefficient γ for an electron confined at a radius $\leq \rho$ is given by $\gamma \sim [1 + (\lambda_c/r)^2]^{1/2}$.

In Fig. 4, we plot KE and $|V_{\text{eff}}|$, for $1 F < \rho < 100$ pm, to clearly show the existence of three zones: for $1 F < \rho < 100$ pm.

- (1) For $26.5 \text{ pm} < \rho$, the atomic zone, where $\text{KE} < |V_{\text{eff}}|$.
- (2) For $2.8 F < \rho \leq 26.5 \text{ pm}$, a zone where $\text{KE} > |V_{\text{eff}}|$.
- (3) For $1 F < \rho \leq 2.8 F$, an EDO zone, where $\text{KE} < |V_{\text{eff}}|$.

Remark. In fact, the presence of EDO electrons is not limited to the zone #3, since we found an EDO wave function having a probability density with mean radius at $4.5 F$, because of the very large tail extending far beyond the range displayed in Fig. 3. But here, we only considered the strongly attractive potential V_{eff} , in a simplified semi-classical analysis.

We make the assumption that an increasing containment of electron wave packet is possible.

The start of this increasing containment is possible, because in the atomic zone #1, we have $\text{KE} < |V_{\text{eff}}|$, which can push a (tiny) fraction of the electron wave packet, whose maximum probability of presence is at the Bohr radius, i.e. at $53 \text{ pm} \sim 2 \times 26.5 \text{ pm}$, to move towards the nucleus until 26.5 pm .

But, arrived at 26.5 pm and for reaching the zone #3, the wave packet should have to go through the zone #2, where the repulsive effect of kinetic agitation required to satisfy the HUR is greater than the attractive effect of the potential V_{eff} .

We say the zone #2 forms a *Heisenberg barrier* between the zone #1 and the zone #3. Of course, this Heisenberg barrier is a virtual dynamic barrier, unlike the usual potential barriers. In addition, there is a reversal of roles between potential energy and kinetic energy: in the usual cases, the kinetic energy KE pushes an electron to cross a barrier, while the potential energy Pr is repulsive and prevents the electron from crossing the potential barrier, and if $Pr > \text{KE}$, a pure classical mechanical reasoning prohibits the crossing. Then only a quantum process of tunneling allows a fraction of the amplitude of the wave associated with the electron to cross the barrier.

Here, it is the attractive dynamic potential of V_{eff} that tends to push the electron to cross the barrier for having an increasing containment, whereas the increasing kinetic energy KE due to the containment, a reactive agitation implied by the HUR, tends to push the electron back. And in pure classical mechanical reasoning, if $|V_{\text{eff}}| < \text{KE}$, the containment of the electron should not increase. But we consider an *extension of the quantum tunneling process* to this specific situation, allowing a fraction of the amplitude of the electron wave to cross the Heisenberg barrier to reach zone #3.

If considering $\Delta E = \text{KE} - |V_{\text{eff}}|$, we can find a maximum of ΔE , equal to ~ 17 MeV, at $\rho \sim 5.6$ F. This is the point at which the barrier to orbital stability is greatest. We plot the curve of ΔE in Fig. 5 for $2.8 \text{ F} < \rho < 27 \text{ pm}$.

5.2. Tunneling through the Heisenberg barrier

To compute a possible tunneling, we use the WKB (*Wenzel–Kramers–Brillouin*) approximation [32,33] in one dimension, similar to the calculation of the Gamow astrophysical factor [34].

We put $K(\rho) = (2m\Delta E)^{1/2}$, where $\Delta E = \text{KE} - |V_{\text{eff}}|$. Note that $K(\rho)$ has physical dimension of momentum. We plot the curve of $K(\rho) \times 10^{21}$, for $2.8 \text{ F} < \rho < 27 \text{ pm}$ in Fig. 6 (the multiplicative factor 10^{21} is only used to simplify the writing of values on the vertical axis). We can remark the similarity of the shape of curves in Figs. 5 and 6.

Then, we compute $Q = \int_{\rho_0}^{\rho_1} K(\rho) d\rho$, where $\rho_0 \sim 2.8 \text{ F}$, $\rho_1 \sim 27 \text{ pm}$, and we put $w_{\text{exp}} = Q/\hbar = 5.65$ which is a dimensionless number. Note that the integral Q of $K(\rho)$ corresponds to the blue area (divided by 10^{21}) below the curve of $K(\rho)$.

The weakening factor of the electron wave amplitude is given by $w \sim e^{-w_{\text{exp}}} \sim 0.003$. So, the electron presence probability is $P = w^2 \sim 9 \times 10^{-6}$. We interpret this result by saying that the general wave function of an 1S electron orbital could be a *linear combination* of EDO state and atomic ground state, with amplitude coefficient $\lambda_{\text{EDO}} \sim 0.003$.

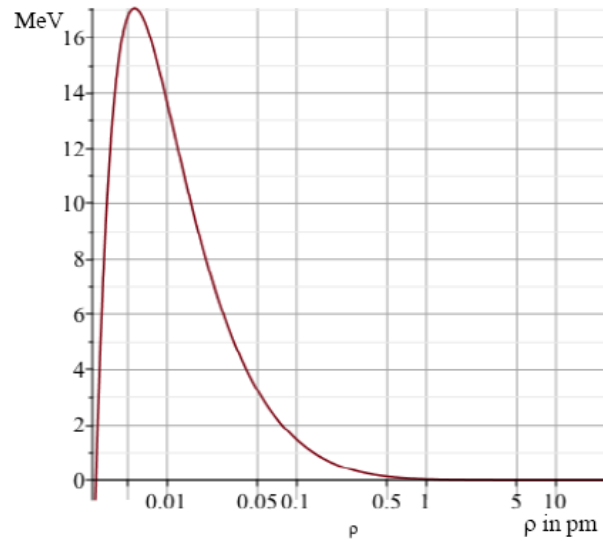


Figure 5. Semilogplot of ΔE , the energy of the Heisenberg barrier, for $2.8 \text{ F} < \rho < 27 \text{ pm}$.

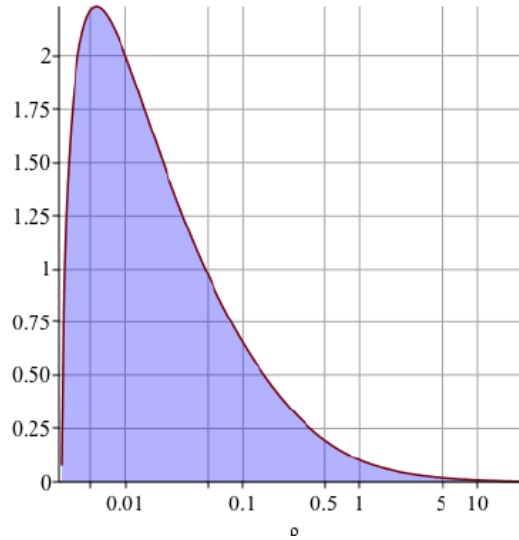


Figure 6. Semilogplot of $K(\rho) \times 10^{21}$ for $2.8 \text{ F} < \rho < 27 \text{ pm}$.

Remark. In [35], the authors also consider that a general solution of the Dirac equation for an electron (or a muon) bound in an atom is a linear combination of the regular (usual) solution and an extra solution, usually neglected; Indeed, this latter solution is eliminated when considering a point-like nucleus; but, it becomes acceptable when taking into account the size of the nucleus, which eliminates the singularity at the origin. Nevertheless, in their numerical results on many atoms, they do not provide the coefficients of linear combinations but the energy shifts due to the size of the nucleus, which is the purpose of their work.

6. Conclusion and Prospect

- (1) Semi-classical simulations carried out in our previous works allow us to solve questions about EDOs as solutions of the Dirac equation with finite nucleus. Indeed, while making semi-classical analysis and computation, we showed the following results:
 - (a) For an electron confined near the nucleus, the HUR requires a strong containment energy but allows us to determine a value for the relativistic γ .
 - (b) We know that the *EDO solutions are highly relativistic*, which is an *important result for LENR*, and as a consequence, the *magnitude order of KE* can be in the 100 MeV range
 - (c) The effective potential, V_{eff} , a relativistic correction of the Coulomb potential deduced from relativistic quantum equations (Dirac or Klein–Gordon equations), can confine deep-orbit electrons within the nuclear region.
 - (d) For a deep electron having an LME and respecting the HUR, we can compute the relativistic coefficient γ , the total energy TE, the kinetic energy KE and the binding energy BE, at the radius r of the LME.

While going back to EDO solutions of Dirac equation for atomic H, by considering a finite nucleus:

- (i) We can recalculate the radial wave functions of Dirac EDO solutions and determine the correct energy level E associated with the radial quantum number n' , and moreover we can compute the coefficient γ , and BE for electron at the mean radius $\langle r \rangle$ of the probability density distribution. So, we solve Problems #2 and #3 (Section 2.2.3, *Obtained results and discussion on imperfections*)
 - (ii) Moreover, we obtain wave functions with smooth continuous shapes and having continuous derivatives everywhere i.e., we solve Problem #1.
- (2) (a) Nevertheless, the Dirac equation seems to provide an EDO solution for each value n' of the radial quantum number, whereas semi-classical computations that do not include resonances between electron-orbital and emitted-photon frequencies as described in [36], give only a single EDO solution. On the one hand, this behavior difference between the quantum equation and semi-classical results also happens for regular solutions: semi-classical computation of electron LME in H atom, carried out while considering only the total energy, provides only the ground (Bohr) state, while a quantum equation, e.g. the Schrödinger equation provides all the excited states, corresponding to increasing values of the main quantum number n (involving the angular quantum number l , as $n = n' + l + 1$). On the other hand, unlike the regular solutions while considering Dirac EDO wave functions, the mean $\langle r \rangle$ radius of the probability radial density distribution decreases when the radial number n' increases. As a consequence, and since $\langle r \rangle$ decreases on a bounded interval, the sequence $\langle r \rangle (n')$ of the values of $\langle r \rangle$ as function of n' , has an accumulation point when n' tends towards infinity. In other words, it means that for high values of n' , the wave function solutions are practically and physically indistinguishable. The meaning of this situation would require further physical interpretation. Can we say that because of quantum fluctuations, from a certain integer N to be defined, all the solutions for $n' > N$ are confounded, and that finally there is only a finite number N of solutions?
- (b) Another question about the Dirac solutions arises, when comparing the characteristic energy parameters of these solutions and those of the semi-classical computations: it seems that semi-classical solution, with LME at radius $r \sim 1.4$ F, is closer to the Dirac solutions for $n' = 2$, where $\langle r \rangle \sim 1.13$ F than the one for $n' = 1$, where $\langle r \rangle \sim 4.5$ F. Of course, we know the Dirac results are dependent on a somewhat arbitrary choice of the junction radius R between inside and outside the nucleus. But even with reasonable decrease of R , we still have a significant gap between the semi-classical solution and the Dirac solution for $n' = 1$: for example, by putting $R = 0.84$ F, i.e. < 0.87 F, which is at the present time the official value of charge radius of the proton, we obtain a mean radius $\langle r \rangle \sim 3.95$ F for $n' = 1$. And on another hand, despite many semi-classical calculations with various combinations of potentials, we never found an LME at a radius $r > 2$ F. The question therefore arises as to *what the solution for $n' = 1$ physically represents, if it is not the basic EDO state?*
- (3) In Section 5, we only began to address the issue of EDO population, by using the WKB approximation for tunneling from atomic state to EDO state. On one hand, the WKB method has been applied in dimension one, when it would make more sense to do it in dim 3. For the time being, various attempts in this direction have not led to realistic results, and the question remains to be addressed.

On another hand, a possible lead would be to look for physical parameters in condensed matter, likely to increase the tunneling toward EDO states. Finally, it should be noted that the analysis carried out in Section 5.1 allows us to give an answer to a legitimate question posed by the referee: why all hydrogen atoms in the Universe (and this is about 74% of all atoms in the Universe) do not spontaneously transfer from standard states to these super-deep levels?

Indeed, we can reasonably expect that the existence of the Heisenberg barrier prevents the electron from *spontaneously* transferring from standard states to super-deep levels. This also answers the naïve question

encountered in forums: *why the electron does not fall into the nucleus?*

- (4) Finally, LENR features such as energy transfer with neither gamma radiation nor energetic particles, requires *enhanced internal conversion*. So, we study possible connections between highly energetic deep electrons and nuclei, hadrons and quarks.

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