



Research Article

Basis for Electron Deep Orbits of the Hydrogen Atom

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Abstract

In this paper, we look into the difficult question of electron deep levels (EDLs) in the hydrogen atom. Acceptance of these levels and, in particular, experimental evidence of their existence would have major implications for the basis for cold fusion and would open up new fields of femto-physics and -chemistry. An introduction shows some general considerations on these orbits as “anomalous” (and usually rejected) solutions of relativistic quantum equations. The first part of our study is devoted to a discussion of the arguments against the deep orbits and for them, as exemplified in published solutions. We examine each of the principal negative arguments found in the literature and show how it is possible to resolve the questions raised. In fact, most of the problems are related to the singularity of the Coulomb potential when considering the nucleus as a point charge, and so they can be easily resolved when considering a more realistic potential with finite value inside the nucleus. In a second part, we consider specific works on deep orbits, named Dirac Deep Levels (DDLs), as solutions of the relativistic Schrödinger and of the Dirac equations. The latter presents the most complete solution and development for spin 1/2 particles, and includes an infinite family of DDL solutions. We examine particularities of these DDL solutions and more generally of the anomalous solutions. Next, we analyze the methods for, and the properties of, the solutions that include a corrected potential inside the nucleus, and we examine the questions raised by this new element. Finally, we indicate, in the conclusion, open questions such as the physical meaning of the relation between quantum numbers determining the deep levels and the fact that the angular momentum seems two orders-of-magnitude lower than the values associated with the Planck constant.

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1. Introduction

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

- the arguments in favor of the deep orbits have become progressively more mature by the use of relativistic quantum tools for a full three-dimensional description of the system;
- by accepting the reality of a non-singular central potential within a nuclear region, many mathematical arguments against anomalous solutions of the relativistic equations no longer pertain;
- numerical evaluation of the relativistic equations are now detailed and available for interpretation of the models, their implications, and their predictions;
- hydrogen atoms, including deuterium, with electron deep orbits (femto-atoms) can contribute to the understanding of: processes of cold fusion inside condensed matter, the avoidance of nuclear fragmentation in $D-D \rightarrow {}^4\text{He}$ fusion reactions, and a means of increasing the rate of energy transfer between an excited nucleus and the surrounding lattice;
- and, above all, recognition of these levels opens up a whole new realm of atomic, nuclear, and subatomic-particle physics as well as nuclear chemistry.

There are various theoretical ways to define a state of the hydrogen atom with electron deep level (EDL) or deep Dirac level (DDL) orbits. In the following, we denote $H^\#$ as any state of hydrogen atom with EDL orbits. Some authors use the term *hydrino* for denoting the $H^\#$ states owing to the work of [1] on the hypothetical existence of H atoms with orbit levels under the Bohr ground level and where the values of orbit radii are fractional values of the Bohr radius. Here, we do not use this term, a physical concept specifically attached to the cited work, because it is not deduced from (standard) quantum equations, while we essentially consider the states $H^\#$ obtained by the methods of relativistic quantum physics. With the quantum equations habitually used in the literature for computing the bound states of the H atom, we can note that there is in general a crossroad with a choice of value or a choice of sign for a square root in a parameter. According to which path is chosen, the resolution process leads either to the usual solution or to an unusual one called an “anomalous” solution; one that is rejected in the Quantum Mechanics textbooks.

In our present study, we note that a $H^\#$ solution is always an anomalous solution but *every anomalous solution is not a $H^\#$ solution*. For example, the anomalous solution also contains the regular energy levels of *anti-hydrogen*. We will see below that it is easy to recognize $H^\#$ solutions, if we have an expression of the anomalous solutions obtained by an analytic method.

A solution provides the eigenvalues of the Hamiltonian, representing the total energy of the electron, in the form of a family of quantized energy levels depending on quantum numbers. We consider only relativistic equations because, in the deep level orbits considered here, the electrons are relativistic. Indeed, we can make a quick computation:

In [2] the authors plot the curve of the normalized electron density of the deep orbit wavefunction corresponding to the ground-state DDL orbit ($-2s$), and this curve has a peak for a radius equal to ~ 1.3 fm. By using the formula of the Coulomb energy potential $CP = -\alpha\hbar/r$, we can calculate $|CP| \sim 1.09$ MeV for this deep orbit. On the other hand, an electron on this orbit has a potential energy equal, in absolute value, to $\gamma mv^2 = |CP| \sim 1.09$ MeV, where v is the electron velocity. From this, we can deduce $v = 2.75 \times 10^8$ m/s, $\beta \sim 0.91$ and $\gamma \sim 2.5$ confirming that the electron is actually relativistic.

The total energy E corresponding to a regular solution in a non-relativistic form for a bound state electron is expressed in negative value and $|E| \ll mc^2$. In relativistic form, the rest mass of the electron is included and, for atomic electrons, $E \sim mc^2(1 - \varepsilon)$. Here $\varepsilon \ll 1$ and depends the coupling constant α and on quantum numbers. We can recognize a $H^\#$ solution, if the relativistic total energy is of the form $E \sim mc^2\varepsilon$.

As the movement of the electron is in a central field, its eigenstate equation is usually written in spherical coordinates and so it can be decomposed into a part depending on angular parameters θ, φ , and another part, a radial equation. The equation on angular parameters has for solutions the spherical harmonics $Y(\theta, \varphi)$ and the wavefunctions $\psi(r, \theta, \varphi)$ verify $\psi(r, \theta, \varphi) = R(r)Y(\theta, \varphi)$, where $R(r)$ is solution of the radial equation (here we omitted the usual quantum numbers indexes). The expression of the wavefunction can take a more complex form, as e.g. for the Dirac equation, but in any case only the radial part can raise questions. Thus, we consider the reasoning on the radial equations and on the radial wavefunctions.

2. Discussion on the Arguments Against the $H^\#$ States

Here, we classify our reflections according to the arguments found in the literature against the existence of these special states of the hydrogen atom and we discuss these arguments.

2.1. The wavefunction can have a singular point at the origin

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

- one factor is a decreasing exponential $\exp(r)$ such that $\exp(r) \rightarrow 0$ when $r \rightarrow +\infty$,
- another one is $\propto 1/r^s$ with s a real number, due to the form of the Coulomb potential,
- and there can be a further one in polynomial form.

In the case of the “anomalous” solutions, the exponent s of the factor in $1/r^s$ is $s > 0$, then the radial function $R(r) \rightarrow \infty$ when $r \rightarrow 0$ and the wavefunction $\psi(r, \theta, \varphi)$ does not obey a boundary condition. This problem comes from the expression of the Coulomb potential in $1/r$. Some authors of $H^\#$ solutions remove this trouble by saying that the classical expression of the central potential is a good approximation for the bound state of a single electron atom, but considering the nucleus as a mathematical point is an unphysical abstraction. In fact, the Coulomb approximation in $1/r$ of the central potential generated by the nucleus is suitable if the electron is not too near the nucleus.

At this point, many authors do not consider a non-singular potential and stop without further development of the anomalous solution; but others work on this subject in expressing corrected potentials in the close vicinity of the nucleus, as e.g. in [2].

That is an actual enhancement of the theory, but it unfortunately entails extra difficulties. Indeed, there are no serious difficulties for defining the weakening of the electrical potential very near the charge radius of the proton and inside it. But problems arise when wanting to find solutions of the equations by taking into account the chosen potential in the neighborhood of the nucleus. Let P_n be this potential, then there are two possible procedures to use P_n :

- (1) To solve the equation with the Coulomb potential and to find a first solution S_1 , then to solve the equation with P_n and find a second solution S_2 near and inside the nucleus, and finally carefully connect S_1 and S_2 in a suitable manner: continuity conditions and even conditions on derivatives at the interface of both potentials.
- (2) In the case where the solution S_1 implies the bound electron is at the contact of the proton or deeper, we can think S_1 is rather erroneous. Then, one should solve the equation directly with the whole rectified potential from 0 to $+\infty$.

2.2. The wavefunction ‘cannot be square integrable’

In this case, the wavefunction cannot be normalized in the entire space and it does not obey a boundary condition for the bound states. This case results essentially from the behavior of the wavefunction ψ at the origin and not for

$r \rightarrow \infty$. To be normalized, the wavefunction has to satisfy $||\psi(r, \theta, \varphi)|| < +\infty$. As the Jacobian of the transformation from Cartesian to spherical coordinates is $J = r^2 \sin \theta$, we have

$$||\psi(r, \theta, \varphi)|| = \int |\psi|^2 \sin \theta r^2 d\theta d\varphi dr = \int |Y(\theta, \varphi)|^2 d\Omega \int |R(r)|^2 r^2 dr, \quad \text{where } \Omega \text{ is the solid angle.}$$

Since the spherical harmonics are normalized, we have only to verify $\int |R(r)|^2 r^2 dr < +\infty$. In fact, the behavior of $|R(r)|^2 r^2$ at infinity does not make any difficulty, because the leading factor, which induces ψ to vanish, is a decreasing exponential factor. Thus, only the behavior of $|R(r)|^2 r^2$ at the origin can be a problem.

Here, we can cite the work of Naudts [3], where a $H^\#$ state is found by using the Klein–Gordon (K–G) equation and the corresponding solution is square integrable. The author derives in one step the K–G equation for the bound electron of the hydrogen atom from the time-dependent Schrödinger equation by introducing the relativistic formulation of the energy. We recall this process in a more explicit way in order to more clearly see what are the implications and the limitations of the K–G equation.

- The relativistic total energy of a free particle of mass m is given by the equation $E^2 = \mathbf{p}^2 c^2 + m^2 c^4$.
- If we consider that an electron of charge e is submitted to an exterior electromagnetic field defined by a scalar electric potential φ and a vector potential $\mathbf{A}$ in covariant form, then the momentum vector $\mathbf{p}$ becomes $\mathbf{p} - e\mathbf{A}$ and the energy scalar E becomes $E - e\varphi$. By substituting in the previous energy equation we obtain $(E - e\varphi)^2 = (\mathbf{p} - e\mathbf{A})^2 c^2 + m^2 c^4$. However, as the electron is in a static Coulomb potential generated by the central proton, we have $\mathbf{A} = 0$ and $e\varphi$ is equal to $V = -e^2/r = -\alpha c\hbar/r$, where α is the coupling constant, also called the fine-structure constant, equal to $\sim 1/137$.
- Finally, we apply the canonical quantization principle, by expressing E and $\mathbf{p}$ by differential operators:

$$E \rightarrow i\hbar\partial_t, \quad \mathbf{p} \rightarrow i\hbar\nabla.$$

Then the equation energy becomes the K–G equation for the electron in the hydrogen atom, as written in the cited paper:

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

where $\psi(r, t)$ is a time-dependent radial wavefunction and m the rest mass of the electron. Historically, this equation was called the *relativistic Schrödinger equation*. In fact, the gauge invariance has been applied in the hypothesis of the Fock minimal coupling [4], so this equation describes the evolution of a relativistic electron in an exterior electromagnetic field [5].

Naudts then tries an ansatz with a function

$$\psi(r, t) = e^{i/\hbar Et} r^{-l} e^{-r/r_0}$$

solution of the equation with the hypothesis $l < 3/2$ and $r_0 > 0$ (here the parameter l does not represent the angular momentum). The condition on the l guarantees the behavior of $|\psi(r, t)|^2 r^2$ at the origin and $r_0 > 0$ its behavior at the infinity, in order for the wavefunction solution to be *square integrable*. The resolution leads to an equation to be satisfied by the parameter l : $l^2 - l - \alpha^2 = 0$ with solutions

$$l = \frac{1}{2} \left(1 \pm \sqrt{1 - 4\alpha^2} \right).$$

We can see a possible choice of sign $\pm$ before the square root. In both cases, the constraint on l is satisfied, i.e. $l < 3/2$. The choice of the negative sign leads to a regular solution that corresponds to the ground energy level associated with the usual quantum number $n = 1$. Indeed the value of the total energy is

$$E \sim mc^2 \left(1 - \frac{\alpha^2}{2} \right)$$

and thus the binding energy is equal to

$$\text{BE} \sim -mc^2 \frac{\alpha^2}{2} = -13.6 \text{ eV}$$

and the orbit radius r_0 is equal to 53 pm. If the positive sign is chosen, the obtained solution is a $H^\#$ state, with total energy very low, $E \sim mc^2 \alpha \sim 3.73 \text{ keV}$. That means a high value for the binding energy, since $\text{BE} \sim mc^2(\alpha - 1) = -507.3 \text{ keV}$.

Naudts calculates excited states by using an analogous ansatz, but all his excited states are found to correspond to regular states. The only $H^\#$ state obtained is the above one, because he considers only spherically symmetric states. Since the exponent $l > 0$, the origin is a singular point for the wavefunction. Naudts argues against this problem by saying that the nucleus is not a point, but its charge is “smeared” over a distance of about 1 fm. 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 $H^\#$ state.

Some criticism can be raised about the application of the K–G equation for a question concerning a bound electron.

- The most classical criticism concerns the fact that the electron is a fermion, spin $\pm 1/2$, whereas this equation does not take into account the spin and there is no way to introduce the Pauli spin matrices without destroying the Lorentz invariance. On one hand, this trouble is slight in comparison with the benefit of finding a square integrable $H^\#$ solution. On the other hand, it’s the same problem for the classical Schrödinger equation and its use is well accepted for finding the energy levels for the light atoms. Moreover, it is not yet time to worry about fine structure for the $H^\#$ states.
- A more subtle criticism concerns the conservation equation

$$\partial_t \rho + \nabla \cdot \mathbf{J} = 0, \quad \text{where } \mathbf{J} = \frac{\hbar}{2im} (\psi^* \nabla \psi - \psi \nabla \psi^*).$$

For the non-relativistic equation, where $\rho = |\psi|^2$ and represents a probability density, ρ satisfies this equation, so its space-integral is time-independent and $\mathbf{J}$ represents a probability current density. However, from the solutions of the relativistic equation, the only possibility is that ρ be proportional to

$$\frac{\hbar}{2imc^2} (\psi^* \partial_t \psi - \psi \partial_t \psi^*)$$

and $\mathbf{J}$ be proportional to the same expression as above. The occurrence of time derivatives in ρ is due to the presence of a second-order time-derivative in the K–G equation. It can be shown that this expression of ρ can be reduced to $\rho = |\psi|^2$ in the non-relativistic limit. Nevertheless, the expression for ρ , when including time derivatives, is not necessarily positive and thus it cannot be considered as a probability density. However, it is possible to interpret it as a charge density in inserting $e\varphi$ (and $e\mathbf{A}$ for $\mathbf{J}$) as indicated in [6,7], because a charge can be positive or negative. Note that this problem does not exist when using the Dirac equation because it contains only first-order time-derivatives. Regardless, this question does not remove the interest in the $H^\#$ solution found by [3]. Finally we note that, if the singular point at the origin is suppressed, the wavefunction is automatically square integrable.

2.3. The orthogonality criterion cannot be satisfied

The Hamiltonian, which represents the total energy, has to be a Hermitian operator in order for its eigenvalues to have real values. This property leads to the following needed condition: eigenfunctions corresponding to distinct values have to be orthogonal. In [8], de Castro examines the asymptotical behavior of the solutions of the non-relativistic Schrödinger, of the K–G and of the Dirac equations by using the Frobenius series method and by considering the

variations of this behavior as a function of formal variations of the coupling constant α . Then, from the orthogonality condition, he indicates deduced conditions under two different forms for the radial solutions, according to which equation is used:

For the K–G equation:

$$(u_k * (du_{k1}/dr) - u_{k1} (du_k * /dr)) \rightarrow 0 \quad \text{when } r \rightarrow 0, \text{ where } u_k(r) = rR(r).$$

For the Dirac equation, we have a condition on the components

$$f, g : (f_k^* g_{k1} - f_{k1} g_k^*) \rightarrow 0 \quad \text{when } r \rightarrow 0.$$

So, for the K–G case, only the solutions with u “less singular” than $\sqrt{r}$ can satisfy the orthogonality criterion. For the Dirac solution, he finds that only the regular solutions for the components f, g can satisfy the orthogonality. In fact, we can see the orthogonality condition is closely related to the behavior of the radial function at the origin [9], itself related to the behavior of the Coulomb potential at the origin. Therefore, this problem can be resolved by a corrected potential, without singular point at $r = 0$, that corresponds in fact to the physical reality. This point is developed in Section 3.3. We can also note several works [10,11] on self-adjoint extension of operators for potentials with singularity. In particular, the first cited work explicitly shows that, for the K–G equation in the case of the Coulomb potential, the “singular” solutions satisfy the orthogonality condition and satisfy also the boundary condition, i.e.: when $r \rightarrow 0$, $\lim u(r) = u(0) = 0$.

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

It may seem absurd to make changes of a physical constant whose value is in principle given by ‘Dame Nature’. But, it can be very instructive to make this “thought experiment”: to imagine variations of the coupling constant α and to examine the consequence of such variations on the energy parameters of the hydrogen atom. In [12], Dombey points out a very strange phenomenon concerning the $H^\#$ solutions of the relativistic equations: when α decreases and tends towards 0, the binding energy of the electron increases and tends towards its maximum. The author solves the K–G equation in an analytic way leading to a Whittaker’s (second-order differential) equation [13,23] on the radial function and the solution is achieved by transformation into a Kummer’s equation [14,24]. So the radial function has the general form with three factors as we noted in Section 2.1, where polynomials are obtained by fixing some parameters of the confluent hypergeometric series [25] solution of the Kummer’s equation. There is a choice of sign for a parameter occurring in the expression of the energy levels. One choice leads to the regular energy levels, while the other sign leads to anomalous ones, E_N , where N is a positive quantum number:

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

We note the presence of a minus sign before the square root in the denominator of the fraction $\dots 1/2 - \sqrt{\dots}$. For the anomalous ground level E_0 , the author obtains the same expression as the $H^\#$ state energy found by Naudts [3], i.e. $E_0 \sim mc^2 \alpha = 3.73$ keV. We can see the total energy E_0 of the electron decreases when α decreases, which means its binding energy $|BE|$ increases in absolute value. And finally $|BE| \rightarrow mc^2$, the *whole rest mass energy*, when $\alpha \rightarrow 0$.

This strange phenomenon seems to concern only the ground state E_0 because, for $N \neq 0$ we have $E_N \sim mc^2(1 - \alpha^2/2N^2)$ for $\alpha \ll 1$, thus E_N increases when α decreases, which is the “normal” behavior. Of course, we have the same result as the ones obtained in [3] by means of an ansatz, but as we have an algebraic expression resulting from

an analytic process, we can see at least a mathematical reason for discriminating the $H^\#$ solution among the set of the anomalous solutions. The explanation lies in the expression Δ in the denominator,

$$\Delta = N + \frac{1}{2} - \left(\frac{1}{4} - \alpha^2 \right)^{1/2}.$$

Indeed if $N = 0$, then Δ can be reduced to α^2 , for $\alpha \ll 1$, leading to the expression for E_0 above. Nevertheless, in some cases [15] there is an infinite family of $H^\#$ states and all these states have the strange behavior with respect to the coupling constant. Note in [12] the author also examines the solutions given by the Dirac equation in two-space-dimensions and finds the same strange behavior of the ground state, which is a $H^\#$ state, with respect to the coupling constant. In fact, we think this result is obtained in a context of an ill-defined system, uniquely on a pure mathematical basis. From a physical point of view, we can see the coupling constant α is actually entangled with several fundamental constants, in particular the Planck constant, the velocity of the light, and the elementary electric charge. So, modifying α without caution can certainly lead to paradoxical physical results (e.g., letting α go to zero means that the charge does also; thus, there are no bound states and no BE).

Another example, extracted from [16], of this kind of problem concerning a physical constant, in a case where the constraints are simpler: the non-relativistic limit of a relativistic theory can be obtained if one lets c tend to infinity, and thus the relativistic coefficient γ becomes 1 for any speed v . However, if doing this on the Dirac operator in an electro-magnetic field, one has to proceed carefully because of terms as such as mc^2 , which would tend to infinity, and as the term $(e/c)\mathbf{A}$ that would turn off the vector potential $\mathbf{A}$ if c tends to infinity. Then the author is led to develop specific techniques and to define some concepts needed on account of the nature of the so-called c -dependence of the Dirac operators.

3. Deep Dirac Levels (DDL). The Deep Orbits Obtained as Solutions of the Relativistic Quantum Equations

In [15], Maly and Va'vra publish their first article on this subject where they define the concept of Deep Dirac Levels (DDL) for the electronic orbits of the Hydrogen-like atoms. Here we consider only hydrogen atoms. In fact, they use two methods for obtaining these deep orbit levels: the former by means of the relativistic Schrödinger equation, and the latter by the Dirac equation. For both equations, they follow the solution method indicated in [6]. We emphasize the use of the Dirac equation.

3.1. Solutions obtained with the relativistic Schrödinger equation

After separation of the radial equation, one introduces an ansatz $R(\rho) = \rho^s e^{-\rho/2} L(\rho)$ into the radial equation, $L(\rho)$ 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 . New parameters are defined to obtain a pure numerical second-order differential equation in $L(\rho)$. One shows that the eigenvalue energy E of the Hamiltonian is defined by the following expression: $E = mc^2[1 - (\gamma^2/\lambda^2)]^{-1/2}$, where λ is a numerical parameter of the equation and $\gamma = Z\alpha$, α being the coupling constant. It is in fact the Sommerfeld relation.

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

$$s = -\frac{1}{2} \pm \left[\left(l + \frac{1}{2} \right)^2 - \gamma^2 \right]^{1/2}.$$

It is the “crossroad” condition indicated at the beginning of this paper. When taking the positive sign in the expression of s , we obtain the usual solution for the electronic energy levels. This choice is taken because with the negative sign we have $s < 0$ for any $l > 0$ and thus the radial wavefunction R tends to infinity when ρ tends to 0 because of the exponential term ρ^s . Note that for $l = 0$, we also have $s < 0$, even when taking the positive sign. But in this case, for small Z and as $\gamma \approx Z/137$, $\gamma^2 \ll 1$ and s is close to zero. Moreover, considering that the nucleus has a size $a \neq 0$, the potential has no singular point near 0 and is finite everywhere. Then, one can show [6] that the solution R is finite at $r = \rho = 0$ and approaches that solution with a singular-point-Coulomb potential when a tends to 0. Nevertheless, as noted in [15] for heavy atoms, the value of γ^2 becomes great enough that s (a negative value) has a non-negligible absolute value for $l = 0$. For example, in the Cs atom, $Z = 55$ and then $s \approx -0.2$. One can observe that for an even-higher- Z hydrogen-like atom, i.e. Fr with $Z = 87$, we have s with an imaginary part; but this fact goes beyond the subject of our paper. As we consider only the H atom, it is sufficient to let $Z = 1$. Anyway, at this point we can consider there is no serious reason for systematically eliminating the so-called “anomalous” solutions obtained with a negative sign in the root s . The argument concerning the physical reality of the finite ($\neq 0$) size of the nucleus can be applied in this case too.

The energy levels corresponding to the “anomalous” solutions are provided by the following expression [15]:

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

where n' is the radial quantum number and l is the angular momentum quantum number. For hydrogen-like atoms, α^2 is simply replaced by $Z^2\alpha^2$. As for the usual solutions, the authors define the total quantum number $n = n' + l + 1$. Then they compute the new energy levels E for all the possible combinations of the quantum numbers $n = 1, 2, \dots, n' = 0, \dots, n - 1$; and $l = n - n' - 1$. The values represented by E are the total energy of the electronic orbitals. The corresponding binding energies, i.e. the values $|\text{BE}| = E - mc^2$, are quoted in several Tables T1 [15] together with the energies of the regular solutions (positive sign in the expression of s) and with the non-relativistic Schrödinger levels for comparison. The results for $Z = 1$ are reproduced in our companion paper [17]. Each table is built-up for a different hydrogen-like atom of the class of the alkali metals. In fact, *every anomalous solution is not a deep orbit: such a deep orbit appears only for $n' = l$* , as emphasized by the authors and as we can see in the tables (where $n = N$, $n' = M$, and $l = L$).

As we have an analytic expression of E , it is possible to find the “secret” of this difference between the three solutions. For doing this, we start from the formula

$$E = mc^2 [1 + (\gamma^2/\lambda^2)]^{-1/2}, \quad \text{where } \lambda = n' + s + 1 \text{ and } s = -\frac{1}{2} - [(l + 1/2)^2 - \alpha^2]^{1/2}.$$

For small Z (here $Z = 1$), we can first show that $\lambda \sim n' - l + \alpha^2/(2l + 1)$. Then we can see that the condition $n' = l$ drastically reduces the expression of λ : $\lambda \sim \alpha^2/(2l + 1)$, and so $\lambda \ll 1$. Carrying this into the expression of E , one can deduce $E \sim mc^2 \alpha/(2l + 1)$. As the fraction $\alpha/(2l + 1) \ll 1$, the binding energy $|\text{BE}|$ is very high and that means the orbit is very deep. So for every l , there is an infinite series of these very deep energy levels with $|\text{BE}| > 507$ keV and an orbit radius of order fm. Concerning the energy levels corresponding to other combinations of the quantum numbers, the tables gives two kinds of results: values similar to the usual energy levels, and values annotated by the authors as “negative energy states, not observable”, appearing for $n' > l$. Finally, we can note that for $n' = l = 0$, for the relativistic Schrodinger case, the binding energy $\text{BE} = -507$ keV, in agreement with the result found in [3] for the energy of the anomalous solution. Moreover the necessary condition, $n' = l$ for the EDL orbits, explains the negative result of the same author concerning the “excited” states ($n' > 0$), because Naudts considered only the case of null angular momentum for the deep-levels.

3.2. Solutions obtained by means of the Dirac equation

The Dirac equation is certainly a cornerstone of modern physics: reconciling quantum physics and special relativity with success, accounting for spin of particles, and having the historical source of the concept of anti-particle even before their actual discovery. It is copiously handled in the literature, e.g. in [4, 6, 7, 18]. Essential features of the Dirac equation and its solutions can be found in [9].

3.2.1. Determining the DDL solutions

Maly and Va'vra use the method developed in [6], where the “crossroad” condition is the sign of a parameter

$$s = \pm \sqrt{(k^2 - \gamma^2)}$$

appearing during the solution process. If choosing the sign “–”, one obtains the expression E of the energy levels for the anomalous solutions

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

The radial quantum number n' can take any positive value 0, 1, 2, ... The quantum number k , eigenvalue of the specific Dirac operator K , is related to the total angular momentum (now including the electron spin). It can take values $\pm 1, \pm 2, \dots$ but not the value 0. Indeed, as K satisfies $\hbar^2 K^2 = \mathbf{J}^2 + \frac{1}{4}\hbar^2$, we can see that k cannot be null, but we can give also a more “physical” argument to understand this fact. In the radial equation, there is a term in k/r playing the role of a repulsive angular momentum barrier that prevents the “fall to the center.” It is like the “effective potential” $l(l+1)/r^2$ appearing in the non-relativistic radial Schrödinger equation. One also defines the main quantum number to be $n = n' + |k|$.

The authors built tables of the binding energies for combinations of the Dirac quantum numbers n' and k appearing in the expression of E , plus the main (or total) quantum number n and the orbital quantum number l . This latter is connected to k by the relation $l = k - 1$, if $k > 0$, else $l = -k$. These Tables T2 also include the hydrogen-like atoms of the alkali class. Here we consider only the hydrogen tables and $k > 0$. ($n = N$, $n' = M$, $k = K$, and $l = L2 = -k$ (used with $k < 0$) for the Dirac levels.) Here again, *every energy level is not a DDL, but only those computed for $n'(= M) = k$* . The mathematical explanation is similar to that for the Schrödinger equation: we can show that the energy values E_D of the DDL orbit satisfy $E_D \sim mc^2 \alpha / 2k$. So, we can see that there is an infinite series of DDL solutions.

Now, we consider the expression $E_S \sim mc^2 \alpha / (2l + 1)$ obtained in the Schrödinger case. Here, the indices D and S refer to the Dirac equation and Schrödinger equations, respectively. While comparing the expressions of E_D and E_S , we can verify the slight shift between the values of E_D and E_S , i.e. $E_D > E_S$ and thus $|\text{BE}_D| < |\text{BE}_S|$, for the equivalent levels determined by n' and thus by $k = l$. For example, for $n' = 1$, the tables displays $\text{BE}_S = 509.8$ keV while $\text{BE}_D = 509.1$ keV. Note that the first deep orbit energy $\text{BE}_S \sim -507$ keV, for $n' = 0$, has no equivalent in the “Dirac table” of the same atom, because the Dirac number k cannot be null. The differences between E_D and E_S is certainly due to the corrective term of *spin-orbit* energy included in the Dirac Hamiltonian and associated with the spin precession. For the regular solutions, there is a smaller total spread in energy of fine structure levels [6] than for the Schrödinger solutions. In fact this corresponds to a slightly bigger TE and thus implies a slightly smaller $|\text{BE}|$. Moreover, we can think this energy shift is much more appreciable at the deep level.

3.2.2. Some particularities of the DDL solutions

In considering $E_D \sim mc^2\alpha/2|k|$ for the total DDL energy, we can see that E_D decreases when k increases. Since the total quantum number $n = n' + |k|$, and $k > 0$, we can write $E_D \sim mc^2\alpha/n$. Thus when n increases, the binding energy $mc^2[1 - \alpha/n]$ increases. So, the variation of the binding energy as a function of the principal quantum number n is the *inverse* of the case for the regular solutions. This fact raises a question: what is the variation of the mean orbit radius as a function of the quantum number n (or k)? It seems this question has never been mentioned, much less addressed. We think the most logical answer, based on the results of [15], should be the following: when n increases, the binding energy increases. That is possible only if the electron moves nearer to the nucleus, so the mean orbit radius decreases. A coarse computation seems to lead to the same hypothesis and a remark in ([2], p.61), the next paper of the authors cited here, corroborates this hypothesis. Under these conditions, we assume that the mean radius corresponds to a charge-accumulation area in orbitals close-about the charge volume of the nucleus in more circular (or spherical) orbits. Of course, only a computation based on the variations of the quantum electron density could determine the correct result. This can be the object of a further paper. Another question leading to further study is: how to physically interpret the fact that DDL orbits appear only when the quantum number n' and k are equal?

3.3. The deep orbits obtained by considering a corrected potential near the nucleus

3.3.1. DDL orbits with a finite potential inside the nucleus

After their earlier work [15], Maly and Va'vra produced a second paper [2] on DDLs where, in particular, they estimate the size of the DDL atoms. They used another method ([19], p.195) for the Dirac equation solution. This method, using similar ansatz, transforms the system of coupled first order differential equations on the radial functions into a second-order differential equation, a Kummer's equation. The general solutions of this equation take the form of confluent hyper-geometrical series, requiring suitable convergence conditions. Of course, there is always the same "crossroad" parameter s that determines the DDL solutions when $s < 0$. In order to make accurate calculations of the size of the DDL atoms, the authors consider that the nucleus has finite dimension, taking into account a finite specific potential inside the nucleus, and they look for the wavefunctions inside the nucleus. Then they show that it is possible to normalize and to "connect" both solutions (outside and inside the nucleus) at a conventional value R_0 of the nucleus, not indicated in the paper. Because of the wavefunctions inside the nucleus, we can show that the global wavefunctions satisfy the orthogonality condition (Section 2.3).

From the couple of radial functions f and g found outside the nucleus, Maly and Va'vra [2] compute the electron density (Eld) outside the nucleus by the formula

$$\text{Eld} = 4\pi r^2(|f|^2 + |g|^2)$$

and they deduce the mean orbit radius

$$\langle r \rangle = A_0 \int_0^\infty r \text{Eld} dr,$$

where A_0 is a normalization constant. They plot curves of Eld for various atoms, for regular and for DDL orbits. In particular, in their Fig. 2 [2], they give the curves of Eld for DDL orbits corresponding to the Dirac quantum number $k = +1$, for H and Li (as hydrogen-like) atoms. For H, the energy level is ~ -509.1 keV, while for Li (with one electron on DDL) it is ~ -505.4 keV. The authors say that the peak of Eld corresponds to the radius of the nucleus. The peak occurs for $r \sim 1.3$ fm. After this, they propose mechanisms of atomic transitions to the DDLs and suggest chemical behaviors of the DDL atoms that, in fact, could behave almost as neutral particles. This would explain the

difficulty in detecting them. Finally, they report experimental results such as calorimetry and radiation detection. This is beyond of the scope of our present paper.

3.3.2. Techniques used when considering a finite potential inside the nucleus and criticism

When considering a finite potential inside the nucleus, there are three stages for finding the solution.

First, the solution is computed outside the nucleus with the Coulomb potential, but with considering the radius $r > R_0$, where R_0 is near the “charge radius” of the nucleus. For example, if we consider the hydrogen atom, the nuclear-charge radius is ~ 0.87 fm. In [20], R_0 is computed for a nucleus of mass number A by means of the formula $R_0 = r_0 A^{1/3}$, where $r_0 = 1.2$ fm.

Next, the solution is computed inside the nucleus, with a chosen potential which is an approximation physically suitable for the problem. For example, one can use, as in [2,18], the Smith–Johnson potential that corresponds to a uniformly distributed spherical charge, i.e.

$$V(r) = - \left[\frac{3}{2} - \frac{1}{2}(r^2/(R_0)^2) \right] Ze^2/R_0,$$

or simply a constant potential, or more complex ones.

Finally, let $g_i(r)$ be the inside solution and $g_o(r)$ be the outside one, both have to be correctly “connected” at $r = R_0$. More precisely, if the initial equation(s) is (are) of differential order 2 as the Schrödinger equation, we have to satisfy the continuity condition for the functions $g_i(R_0) = g_o(R_0)$, and also for their first order derivative, i.e. $g'_i(R_0) = g'_o(R_0)$. In fact both conditions can be combined into a “matching” equation of the form $g'_i(R_0)/g_i(R_0) = g'_o(R_0)/g_o(R_0)$. Of course, the normalization of the whole wavefunctions defined for $r \in [0, +\infty)$ has to be carried out after matching.

An interesting criticism is found in [20] where the Dirac “anomalous” solution is not rejected, but is in a way combined with the regular one in a linear combination with coefficients to be computed to satisfy the continuity conditions at the matching radius. From the result, we can see the anomalous solution is involved with a very small ratio, as a little perturbation. We observe that the authors use a solution method based on the use of a Whittaker’s [13] (second order) differential equation. The solutions include confluent hypergeometric series as factors of exponential functions, in particular ρ^s , which does not diverge at $\rho = 0$ thanks to the finite chosen potential. Nevertheless, if considering both the regular and the anomalous solutions at the same time, a difficulty appears for the convergence of the series when $\rho \rightarrow +\infty$: the convergence condition depends on the sign of the crossroad parameter s . To resolve this difficulty, the authors have to combine both kinds of series in order for the divergences to be exactly balanced, when using asymptotic forms of the series. Then the authors have to unify a parameter E representing the energy, when they verify the continuity conditions at $r = R_0$. Here we can note that, if using the solution method proposed in [6] or in [21], then the convergence of the series is independent of the crossroad parameter s , which greatly simplifies the problem.

The criticism of Deck, Amar, and Fralick [20] about the method used in [2] concerns the lack of dependence on the potential inside the nucleus and on the boundary conditions at the nuclear radius. In fact, matching in a simple way the wavefunction outside the nucleus with a solution inside the nucleus is an approximation that only allows removal of the singularity at the origin. We think that the form of the nuclear potential can have a significant effect on the energy levels, particularly for deep orbits. So, in order to improve the precision of the DDL levels, we suggest the following method: to start from a corrected global potential built by connecting in a smooth way the Coulomb potential outside the nucleus with a chosen nuclear potential [22], then to numerically solve the radial equations with this global potential and to compute the corresponding DDL energies. This could be the object of further work.

Note finally a method indicated in [16,18], which allows one to “regularize” the Coulomb potential without the arbitrariness of the cut-off near the nucleus (in particular with the choice of a radius R_0). This method consists of taking into account the “anomalous” magnetic moment of the electron in the unmodified Coulomb potential, and it can be generalized to other potentials with singularity at the origin. Thaller shows that, in doing this, one modifies the radial Dirac operator written in matrix form to have an additional term $\mu_a \alpha / r^2$ not diagonal, where in natural units $\mu_a = 0.00058$ determines the anomalous magnetic moment of the electron. We cite the author: “this term acts as a repulsive interaction that forces the wavefunction away from the singularity”. In fact, this factor (one of several physical mechanisms that would prevent an electron from reaching $r = 0$ in a $1/r$ potential) is extremely small; nevertheless, it becomes dominant against the attractive diagonal Coulomb term α/r for an electron near the origin. Here, the term “regularize” means that the modified Dirac operator has all the “good” properties for providing counter arguments to all the criticisms analyzed above.

4. Summary, Conclusions, Open Questions, and Future Work

In the first part of this paper, we discussed the principal arguments against deep orbits (DDL) for the H atom and we showed how it is possible to resolve the questions raised. Next we looked at the computational results of Maly and Va'vra [2,15] that produced an infinite set of the anomalous solutions, usually rejected, of the relativistic Schrödinger equation and the Dirac equations.

- We observed that only a subset of these solutions, but an infinite one, corresponds to deep orbits: the ones satisfying the equality between the quantum numbers that determine the values of energy levels, i.e. the radial number n' and the angular number (l for the Schrödinger equation and k for the Dirac equation).
- We saw that the electron binding energy on these DDL orbits, of order 509–511 keV, increases when the angular quantum number increases. This result seems to indicate that the mean radius of the DDL orbits decreases when n' increases. Though it is not explicitly stated by the authors, some remarks in their second paper clearly corroborates this hypothesis, and it seems there is an accumulation zone of the orbits in the neighborhood of the nucleus, near a radius of order 1 fm. Of course only a precise quantum computation of the mean radius as function of n' could confirm this hypothesis.
- Another feature that begs for explanation is the predicted ‘angular momentum’ quantum numbers that are for quantities, which are two orders-of-magnitude lower than the values associated with the Planck constant.
- We also noted that another infinite subset of solutions give energy values very near the regular atomic-electron levels, while the corresponding wavefunctions are not the ones of the regular solutions. This result and the previous one about the quantum numbers, raise questions about their possible physical interpretation.

In seeking the source of the deep orbits and their unique structure, we thought of the situation of the DDL orbits in an extreme **B**- and **E**-field from the binding nucleus. This implies a major strengthening of the several “special” known effects that affect the regular atomic-electron orbits. These include the spin–orbit and spin–spin interactions, the Zitterbewegung, and the Lamb shift. For example, the spin–spin interaction, responsible for the hyperfine structure, and the corresponding quantum number associated could play an important role in the determination of energy shifts. However, the deep levels, discrete and asymptotically approaching a binding energy of 511 keV, are also predicted by the relativistic-Schrödinger (K–G) equation, which does not include spin effects. Therefore, any spin-related contributions must be limited to the Dirac equations.

Since the relativistic-Schrödinger equation does not include spin effects, the remaining feature in common (and one not shared with the non-relativistic-Schrödinger equation) is the relativistic formulation that includes the rest mass of the electron. Both equations predict deep orbits with spin effects as a minor perturbation. We might suggest that there is a ‘hidden’ variable within quantum mechanics that may be associated with relativity (or its formulation in

quantum mechanics). Perhaps there are possible new quantum numbers associated with known physical effects, such as relativistic and field-induced precession and nutation of the electron-spin vector. Nevertheless, the latter are only the perturbation effects, not the main story.

From the analysis of the work [2] on the DDL orbits obtained with a corrected potential near the nucleus and the questions raised about these solutions, we think that a more accurate estimation of the DDL orbit energies and radius should result from a numerical “direct” computation of the radial wavefunction with an improved potential from $r = 0$ to infinity. An alternative to this computation could take into account the anomalous magnetic moment of the electron with unmodified Coulomb potential. Introduction of a Hamiltonian including the nuclear-spin interaction with the DDL electron spin would be necessary to include the spin–spin effect. This has an extremely small effect on the atomic-electron orbits, but should be a major effect on electrons in femto-meter orbits. These questions will be the object of further work.

The conclusions from this paper are as follows:

- the anomalous solution to the relativistic Schrodinger and Dirac equations cannot be rejected if a physically real potential is used;
- even though the electron deep orbits do not have sufficient angular momentum to allow standard quantized orbits, the mathematical solutions to these equations include an infinity of discrete orbits;
- by similarity with the atomic-electron orbital solutions, it would appear that there is another set of electron waves (perhaps only when bound) at the higher frequency associated with the deep orbits.

The final conclusion is a series of questions and comments. Is the major effect producing the electron deep orbits from relativistic-velocity effects or is it some form of symmetry-breaking for deep orbits from mass effects? Is the effect real? What are the equations and their solutions trying to teach us? The anomalous solutions have been rejected because there is no data to prove that they exist. Because the solutions have been rejected, data that might prove the deep levels are rejected, explained away, or used to build different models. Cold fusion provides hundreds of experiments that can be more readily explained by the existence of the electron deep levels. Cold fusion will probably provide the physical material from which the deep levels can be verified. Such material probably already exists (even in 2014) that can uniquely and incontrovertibly prove both cold fusion and the electron-deep-level models.

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