Research Article

Arguments for the Anomalous Solutions of the Dirac Equations

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Abstract

In this paper, we look into the difficult question of electron deep levels in the hydrogen atom. 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 the second part, we consider specific works on deep orbits as solutions of the relativistic Schrödinger and of the Dirac equations, named Dirac Deep Levels (DDLs). 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. We next 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. As a prerequisite to a deep comprehension of the resolution methods, we recall in the appendices some essential elements of the Dirac theory.

1. Introduction

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

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- 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;
- 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 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 one called "anomalous" solution, 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 wave function corresponding to the ground-state DDL orbit ($-2s$), and this curve has a peak for a radius equal to $\sim$1.3 fm. By using the formula of the Coulomb energy potential $CP = -\alpha c\hbar/r$, we can deduce $|CP| \sim 1.09$ MeV for this deep orbit. On the other hand, we can deduce from the fundamental dynamics principle in the relativistic framework, that an electron on this deep orbit has a potential energy equal, in absolute value, to $\gamma m v^2 = |CP| \sim 1.09$ MeV, where v is the electron velocity. The relativistic coefficient γ is equal to $(1 - v^2/c^2)^{-1/2}$. By simple algebraic transformations, we can deduce a quadratic equation on an unknown parameter $V = v^2$. From the positive root of this equation, we obtain $v = 2.75 \times 10^8$ m/s, $\beta \sim 0.91$ and $\gamma \sim 2.5$. These results confirm that the electron is actually relativistic.

Of course, it is possible to obtain anomalous solutions by means of a non-relativistic equation, such as the Schrödinger equation. But in this case the energy levels are the same as the regular ones even if the wave functions are different from the regular solutions. This corresponds to a class of solutions we name "pseudo-regular", obtained also by relativistic equations. This class of solutions is described in Section 3.3.2.

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, $E \sim mc^2(1 - \varepsilon)$, where $\varepsilon \ll 1$ and depends on the coupling constant α and on quantum numbers. For a $H^\#$ solution, 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 eigen state equation is usually written in spherical coordinates and it can be decomposed into a part depending on angular parameters θ, φ, and another part, the 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 the solution of the radial equation (here we omitted the quantum numbers indexes). The wavefunction can take a more complex form, for example when using the Dirac equation, but in any case only the radial part can raise questions. Thus, we consider the reasoning on the radial equations and 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 wave function 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 $\exp(r) \to 0$, when $r \to +\infty$,
- 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 $R(r) \to \infty$ when $r \to 0$ 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.

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 near the charge radius of the proton and inside it, by approximating the nucleus as a uniformly charged sphere. But problems rise when wanting to find solutions of the equations by taking into account the chosen potential for the neighborhood of the nucleus. Let *Pn* be this potential, then there are two possible procedures to use *Pn* :

(1) To solve (analytically if possible) the equation with the Coulomb potential and to find a first solution S1, then to solve the equation with *Pn* and find a second solution S2 near and inside the nucleus, and finally connect S1 and S2 in suitable way, i.e. by taking in account continuity conditions and even conditions on derivatives of both solutions at the interface of both potentials. Moreover, we note it would be preferable to beforehand connect carefully the potentials themselves. This procedure of connection has been used in several works, as, e.g., in [2].

(2) In the case where the solution S1 implies the bound electron is almost at the contact of the proton or deeper, i.e. beyond the chosen radius for the potential interface, then we can think S1 is rather erroneous. In this case, the best procedure would be to solve the equation with the whole rectified potential from 0 to the infinity. Of course such a solution would use numerical tools. Note in the case of a complex equation as the Dirac one,

the potential is taken into account only when arriving at the couple of differential equations on the component functions classically denoted as f and g. Nevertheless, at this point, there was not yet a choice between the regular and the anomalous solutions.

2.2. The wave function can be 'not square integrable'

In this case, the wave function 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 $r \to \infty$

To be normalized, the wavefunction must 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 $||\psi(r,\theta,\varphi)|| = \int |\psi|^2 \sin \theta \ r^2 d\theta \ d\varphi \ dr = \int |Y(\theta, \varphi)|^2 d\Omega$ $\int |R(r)|^2 r^2 \ dr$, where Ω 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 Jan 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 of the K–G equation and what are its limitations.

- The relativistic total energy of a free particle of mass m is given by the following equation:

$$E^2 = \mathbf{p}^2 c^2 + m^2 c^4.$$

- If we consider an electron of charge e, 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 E becomes E - $e\varphi$. By substituting in the previous energy equation we obtain $(E - e\varphi)^2 = (\mathbf{p} - e\mathbf{A})^2 c^2 + m^2 c^4$. But, if the electron is in a central Coulomb potential generated by a 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.
- Finally, by expressing E and $\mathbf{p}$ by differential operators, i.e. $E \to i\hbar \partial_t \ \mathbf{p} \to -i\hbar \nabla$, the energy equation 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*.

- Then the author tries an ansatz with a function

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

with the hypothesis $l < 3/2$ and $r_0 > 0$ (do not confuse l with the usual notation for the angular moment). The condition on the exponent l guarantees the behavior of $|\psi(r, t)|^2 r^2$ at the origin and $r_0 > 0$ its behavior at the infinity. So the wavefunction solution is *square integrable*. The resolution by 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 $\pm$. In both cases, the constraint on l is satisfied: $l < 3/2$. 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 $E \sim mc^2 \left(1 - \frac{\alpha^2}{2}\right)$, thus the binding energy is equal to $BE \sim -mc^2 \frac{\alpha^2}{2} = -13.6$ 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, $E \sim mc^2 \sim$ 3.73 keV. That means a high value for the binding energy, since $BE \sim mc^2(\alpha - 1) = -507.3$ keV.

Naudts calculates excited states by using an analogous ansatz, but they correspond to regular states. The only $H^{\#}$ state obtained is the above one, as he considers only spherically symmetric states, i.e. the zero angular moment states. As the exponent $l > 0$, the origin is a singular point for the wavefunction. Naudts argues against this singularity by saying that the nucleus is not a point, but its charge is "smeared" over a distance of about 1fm. Solving the equation with a smeared out Coulomb potential would produce a solution not diverging at the origin, but with certain minor changes on the $H^{\#}$ state.

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

– 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 $\partial_t \rho + \nabla \cdot \mathbf{J} = 0$, where

$$\mathbf{J} = \frac{\hbar}{2im}(\psi^* \nabla \psi - \psi \nabla \psi^*).$$

For the Schrödinger equation, $\rho = |\psi|^2$, it represents a probability density and satisfies the conservation equation. So its space-integral is time-independent and $\mathbf{J}$ represents a probability current density. But from the solutions of the K–G equation, the only possibility is that ρ be proportional to $\frac{\hbar}{2imc^2}(\psi^* \partial_t \psi - \psi \partial_t \psi^*)$. The occurrences of time derivatives are due to the presence of a second time-derivative in the K–G equation. This expression can be reduced to $\rho = |\psi|^2$ in the non-relativistic limit. But the previous expressions including time derivatives, is not necessarily positive and it cannot be considered as a probability density. In fact, it can be interpreted as a charge density in inserting $e\varphi$ (and $e\mathbf{A}$ for $\mathbf{J}$) as indicated in [4,5], because a charge can be positive or negative. Note that this problem does not exist for the Dirac equation, because it contains only first 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 can be suppressed (e.g. by means of a corrected potential near the origin), the wavefunction is automatically square integrable.

2.3. The orthogonality criterion can be not satisfied

The Hamiltonian, which represents the total energy, has to be a Hermitian operator in the standard quantum mechanics in order for its eigenvalues to have real values. This leads to the following needed condition: eigenfunctions corresponding to distinct values have to be orthogonal. In [6], de Castro examines the asymptotical behavior of the solutions of the non-relativistic Schrödinger, of the Klein-Gordon 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 case of the Schrödinger/Klein–Gordon equation,

$$\left(u_k^* \frac{\mathrm{d}u_{k1}}{\mathrm{d}r} - \frac{\mathrm{d}u_k^*}{\mathrm{d}r} u_{k1} \right) \to 0, \quad \text{when } r \to 0, \text{ where } u_k(r) = r R(r),$$

where u_k and u_{k1} are two different eigenfunctions, and the same thing for f_k, f_{k1} and g_k, g_{k1}.

For the case of the Dirac equation, we have a condition on the upper and lower components denoted f, g in usual notation [4]:

$$\left(f_k^* g_{k1} - f_{k1} g_k^* \right) \to 0, \quad \text{when } r \to 0,$$

where u_k and u_{k1} are two different eigenfunctions, and the same thing for $f_k \neq f_{k1}$ and $g_k \neq g_{k1}$.

Next he indicates that for the Klein–Gordon case, only the solution such that u is "less singular" than $\sqrt{r}$ can satisfy the orthogonality criterion. That implies $R(r) \propto r^{-l}$ with $l < 1/2$. And, for the Dirac solution, he finds that only the regular solutions for the components f, g can satisfy the orthogonality, because the condition is $R(r) \propto r^{-l}$ with $l < 1$. So, the problem of the orthogonality is closely related to the behavior of the radial function at the origin, itself related to the singularity of the Coulomb potential at $r = 0$. Therefore, this problem can be resolved by a corrected potential, without singular point at $r = 0$, that corresponds in fact to the physical reality.

We also note several works [7,8] on self-adjoint extension of operators for potentials with singularity. In particular, Nadareishvili and Khelashvili [7] explicitly show that, *in the case of the Klein–Gordon equation with a Coulomb potential, the "singular" (anomalous) solutions satisfy the orthogonality condition and satisfy also directly the boundary condition*, i.e. when $r > 0$, $\lim u(r) = u(0) = 0$.

For the Dirac equation with a Coulomb field, it is more complex. In [9], Thaller uses the notion of essentially self-adjoint operator ([10], p. 256) for potentials with singularity: an operator is essentially self-adjoint if it has an unique extension to a larger domain, where it is self-adjoint. But to satisfy the orthogonality condition and the boundary condition, it is necessary to consider a corrected potential near the nucleus. This point is addressed in Section 3.4.2.

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

It can 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 [11], Dombey points to 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 Klein–Gordon equation in an analytic way leading to a Whittaker's (second-order differential) equation [12] on the radial function and the solution is classically achieved by transformation into a Kummer's equation [13]. So the radial function has the general form with three factors as we noted in Section 2, where polynomials are obtained by fixing some parameters of the confluent hypergeometric series solution of the Kummer's equation. As in the analytic resolution of the Schrödinger 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. Here is the expression of total energy at the level N:

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

The only difference between the anomalous and the regular solution is the presence of a minus sign before the square root in the denominator of the fraction $\ldots \frac{1}{2} - \sqrt{} \ldots$ instead of a plus sign. 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. Now we can trivially 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 very strange phenomenon seems to concern only the ground state E_0 because, for $N \neq 0$, we have

$$E_N \approx mc^2 \left(1 - \frac{\alpha^2}{2N^2} \right) \quad \text{for } \alpha \ll 1,$$

thus E_N increases when α decreases, i.e. the usual behavior. Of course, we have the same result as the ones obtained in [3], but now we have an algebraic expression resulting from an analytic process, so we can see at least a mathematical reason for discriminating the H$^{\#}$ solution among the set of the anomalous solutions. Indeed, the explanation lies in the expression Δ in the denominator, $\Delta = N + \frac{1}{2} - \left(\frac{1}{4} - \alpha^2 \right)^{1/2}$: if $N = 0$, Δ can be reduced to α^2 for $\alpha \ll 1$, leading to the expression for E_0 above. Nevertheless, we see in some cases there is an infinite family of H$^{\#}$ states and all these states have the strange behavior w.r.t. the coupling constant. It is the case for example in [14], where the relativistic Schrödinger/Klein–Gordon equation is solved by using a more direct method as in [4] providing an infinity of H$^{\#}$ states. An analogous result is obtained by means of the Dirac equation.

Note in the paper cited above [11] the author 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 much precaution can certainly lead to paradoxical physical results.

Another example, extracted from [9], 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. But if doing this on the Dirac operator in an electromagnetic 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. DDL (Deep Dirac Levels). The Deep Orbits Obtained as Solutions of the Relativistic Quantum Equations

In [14], Maly and Va'vra publish their first article 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 [4]. We give a quick outline of the solution process, explicitly handled in the appendices, and we discuss the solutions. We emphasize the use of the Dirac equation.

3.1. Solutions obtained by [14] with the relativistic Schrödinger equation

This equation has been written in Section 2.2. After separation of the radial equation, one introduces an ansatz $R(\rho) = \rho^s e^{-\rho/2} L(\rho)$ into the radial equation, where R represents the radial wavefunction, $L(\rho)$ 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 in spherical coordinates. As usual, new parameters are defined by combining the initial physical parameters of the radial equation, in order 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: $E = mc^2 \left[1 + (\gamma^2/\lambda^2) \right]^{-1/2}$ 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. From the differential equation in ρ, we have two conditions to satisfy:

(1) $s(s+1) + \gamma^2 - l(l+1) = 0$, when introducing $\rho = 0$ in the equation, where l is the angular moment quantum number,
(2) $\lambda = n' + s + 1$, to obtain the convergence of the series $L(\rho)$, where n' is an integer ≥ 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. Indeed, 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 $\gamma \simeq Z/137$, $\gamma^2 \ll 1$ 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 [4] 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 [14] for heavy atoms, the value of γ^2 becomes great enough that s (< 0) 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 a 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:

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

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 (by using the formula in γ and λ) for all the possible combinations of the quantum numbers $n = 1, 2, \ldots$; $n' = 0, \ldots, n-1$; and $l = n - n' - 1$. Of course, the values represented by E are the total energy of the electronic orbitals.

The corresponding binding energies, i.e. the values $BE = E - mc^2$ are quoted in several tables (Table 1), 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 Appendix A.8.

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 Tables 1 and 2 (where $n = N$, $n' = M$, $l = L$).

As we have an analytic expression of E, it is possible to find the "secret" of this discrimination. For doing this, we start from the formula

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

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, we can next show that the total energy $E \sim mc^2\alpha/(2l + 1)$. As the fraction $\alpha/(2l + 1) \ll 1$, the binding energy $|BE|$ is very high and that means the orbit is very deep. So for every l, $|BE| > 507$ keV, which gives an orbit radius of order fm. There is an infinite series of these very deep energy levels.

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 $BE = -507$ 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, because he considered only the case of null angular momentum.

3.2. Solutions obtained by means of the Dirac equation

3.2.1. *Determining the DDL solutions*

The authors refer to and use the method developed in [4] that we indicate in Appendix A.6. Here is the expression of the anomalous solutions obtained from the regular solutions by changing the sign "plus" by a sign "minus" between n' and the square root, at the denominator of the internal fraction:

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

E depends on two quantum numbers n' and k. The radial quantum number n' can take any positive values 0, 1, 2 … and k is related to the total angular momentum (now including the electron spin). It can take values $\pm 1, \pm 2, \ldots$ but not the value 0. Indeed, from the relation $\hbar^2 K^2 = \mathbf{J}^2 + \frac{1}{4}\hbar^2$ given in Appendix A.4, 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, Appendix A.6, the term in k/r plays 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 well-known non-relativistic radial Schrödinger equation. One also defines the main quantum number to be $n = n' + |k|$.

As was done for the relativistic Schrödinger equation, the authors built tables of the binding energies for combinations of the specific 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 $l = -k$. This Table 2 also concerns the hydrogen-like atoms of the alkali class. Here we consider only the hydrogen tables and $k > 0$. $\left[n = N, n' = M, k = K, \text{ and } l = L2 = -k \text{ (used with } k < 0) \text{ for the Dirac levels} \right]$.

Here again, every energy level is not a DDL, but *only those computed* for $n'(= M) = k$. The mathematical explanation is similar as the case of 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 equation, 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 $|BE_D| < |BE_S|$, for the equivalent levels determined by n' and thus by $k = l$. For example, for $n' = 1$, the tables displays $BE_S - 509.8$ keV while $BE_D - 509.1$ keV. Note that the first deep orbit energy $BE_S \sim -507$ keV, for $n' = 0$, has no equivalent in the "Dirac table" of the same atom, because the Dirac number k cannot be null.

It is quite normal to have differences between these values, because the Dirac Hamiltonian includes the additional corrective term of *spin-orbit* energy (Appendix A. 5), associated with the spin precession, and corresponds, for the regular solutions, to a smaller total spread in energy of fine structure levels [4] than for the Schrödinger solutions. In fact this corresponds to a slightly bigger $|TE|$ and thus implies a slightly smaller $|BE|$. Moreover we think this energy shift is much more appreciable at the deep level.

3.2.2. *Some particularities of the DDL solutions*

In considering the approximate expression, $E_D \sim mc^2 \alpha / 2|k|$ for the total DDL energy deduced from the special condition $n' = k$, we can see that E_D decreases when k increases. Since the total quantum number is defined by $n = n' + |k|$, 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 [14], 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. 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 other energy values provided by the algebraic Expression E

Now we look at the energy values that do not define DDL orbits. To simplify, we consider $k > 0$.

3.3.1. *Negative energies and masses*

Maly and Va'vra [14] indicate that some results in the tables (see also Appendix A. 8) cannot be observed as energy levels in atoms with electrons, because they correspond to "negative energy" states. This situation happens with $k > n'$ for the Dirac case, and for $l > n'$ for the Schrödinger case. We can easily deduce this condition from the expression of E.

Consider only the Dirac case and the process used to obtain the energy expression, as indicated in Appendix A.7. By the end of the process, we have the relation (A.21):

$$2\beta(s + n') = \gamma(\beta_1 - \beta_2) = \frac{2E\gamma}{\hbar c}, \quad \text{where } \beta > 0 \text{ and } s = -\sqrt{k^2 - \gamma^2} = -\sqrt{k^2 - \alpha^2},$$

since here (H atom) we have $Z = 1$. Therefore

$$\sqrt{(k^2 - \alpha^2)} = k\sqrt{\left(1 - \frac{\alpha^2}{k^2}\right)} \text{ and as } \alpha^2 \ll 1, \quad k\sqrt{\left(1 - \frac{\alpha^2}{k^2}\right)} \sim k\left(1 - \frac{\alpha^2}{2k^2}\right), \text{ thus } s + n' \sim n' - k + \left(\frac{\alpha^2}{2k}\right).$$

From (A.21), we can see that E has the sign of the expression $s + n'$. If $k > n'$, then $s + n' \leq -1 + (\alpha^2/2k)$, and as the additive term at right is $\ll 1$, we have effectively $E < 0$. There is a similar verification for the similar relativistic-Schrödinger case.

3.3.2. *Pseudo-regular energy levels*

Here again, we consider only the Dirac case, the Schrödinger case being similar. We can show that, for any couple (n', k) such that $k \leq n'$ and $n' \neq k$, E is not a DDL energy. E is almost equal to the energy of a *regular level* corresponding to the principal quantum number $N = n' - k$. Moreover, for any N given, there is only a very slight value shift that depends on the chosen couple (n', k) verifying $n' - k = N$. This can be observed on the values displayed on the tables of [14]. More precisely, we consider the denominator D of the fraction inside the expression $E(n', k)$. By using the same approximation as above in Section 3.3.1, we can write

$$D = \left[n' - \sqrt{(k^2 - \alpha^2)}\right]^2 \sim \left[n' - k + \left(\frac{\alpha^2}{2k}\right)\right]^2.$$

If we consider the expression $E_R(n'_R, k_R)$ *of a "regular" solution, its inside denominator D_R is very similar to D, with only a changing of sign, i.e.*

$$D_R = \left[n'_R + \sqrt{(k_R^2 - \alpha^2)}\right]^2 \sim \left[n'_R + k_R - \left(\frac{\alpha^2}{2k_R}\right)\right]^2.$$

Now we can see that the value of the energy level $E(n', k)$ is very near any regular level with principal quantum number $N = n'_R + k_R = n' - k$.

Moreover, on account of the term $\alpha^2/2k$ inside D, we can see that for the same value of $N = n' - k$, when k increases then $|E(n', k)|$ decreases and thus the corresponding binding energy $|BE'(N, k)|$ increases. But the variation of E as function of the principal quantum number $N = n' - k$ follows the classical behavior of the regular solutions, i.e. when N increases, then the total energy $E(N, k)$ increases and the shifts induced by k are very small in comparison with the "principal" variation with N. Under these conditions, we can think the mean orbit radius increases with N, as for the "standard" regular solutions. Nevertheless, a question remains: the wavefunctions of the solutions $E(n', k)$ being determined from a parameter s of negative sign, are not the same as the ones of the "normal" regular solutions, especially near the origin. So, we have yet to physically interpret the existence of these *pseudo-regular* solutions of the Dirac equation. This question could be another object of further study.

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

3.4.1. *DDL orbits with a finite potential inside the nucleus*

After their work [14], where the authors defined the DDLs, they continued their study with a second paper [2] where, in particular, they estimate the size of the DDL atoms. For doing this, they start with another method ([15],Vol. II, p.195) for the Dirac equation solution. This method, using similar ansätze, 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. For doing this, they choose a potential derived (by adding a constant) from the Smith–Johnson potential, corresponding to a uniformly distributed spherical charge:

$$V(r) = -\left[\frac{3}{2} - \frac{1}{2}\left(\frac{r^2}{R_0^2}\right)\right]\frac{Ze^2}{R_0}. \tag{4}$$

The radial equations with this potential are solved with a couple of functions g_i and f_i in the following form: $g_i = Ar^{Si-1}G_2(r)$, $f_i = iBr^{Si-1}F_2(r)$, where $F_2(r)$ and $G_2(r)$ have the form of power series

$$G_2 = a_1r + a_2r^2 + \cdots \quad \text{and} \quad F_2 = b_1r + b_2r^2 + \cdots$$

Recurrent formulas lead to some coefficients. For example, for $k > 0$, k being the Dirac angular quantum number, one has $b_1 \neq 0$, $Si = k - 1 \geq 0$, $a_l = 0$. Only the terms of degrees $n \leq 5$ are kept in G_2 and F_2. Then they show that it is possible to numerically 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.

Now, if we considerer a solution (g_i, f_i) "inside the nucleus", the term of minimal degree of the polynomial g_i is k and the one of f_i is $k-1$. So, in the formula used to verify the *orthogonality criterion* (Section 2.3), $(f_k^* g_{k1} - f_{k1} g_k^*) \to 0$ when $r \to 0$, the expression to be considered is a polynomial P having a term of minimal degree $2k - 1$ and thus, for any $k > 0$, P does not contain a constant term. We can deduce that *the corresponding global solution satisfies the orthogonality condition*. Next, if we look at the boundary condition, expressed by $g_i \to 0$ and $f_i \to 0$ when $r \to 0$, we can see this property is verified for any $k > 1$.

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 $Eld = 4\pi r^2 \left(|f|^2 + |g|^2\right)$ and they deduce the mean orbit radius

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

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 reference to ([2], p.63, Fig. 2), they give the curves of *Eld* for DDL orbits corresponding to the 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, that seems rather logical. By looking at the curve, we can see that the peak occurs for $r \sim 1.3$ fm. After this, the authors propose mechanisms of atomic transitions to the DDLs and they 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.

3.4.2. *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, i.e. for 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 only the hydrogen atom, the charge radius is ~ 0.87 fm, and in [16] R_0 is computed for a nucleus of mass number A by means of the empirical 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 what is an approximation physically suitable for the problem. For example, one can use, as in [16,2], the Smith–Johnson potential, 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 $g_i'(R_0)/g_i(R_0) = g_o'(R_0)/g_o(R_0)$. But for a first-order differential equation such as the Dirac equation that leads to a combined system of two first order equations on two radial functions $f(r)$ and $g(r)$, we have only to satisfy the continuity condition. However, this involves four functions, i.e. $g_i(R_0) = g_o(R_0)$ and $f_i(R_0) = f_o(R_0)$ that can be combined into a simple matching condition $g_i(R_0)/f_i(R_0) = g_o(R_0)/f_o(R_0)$. Of course, the normalization of the whole wavefunctions defined for $r \in [0, +\infty)$ has to be carried out after matching.

Some purist criticisms concern the fact that, for some chosen nuclear potential inside, the whole potential $V(r)$ as a function on $[0, +\infty)$ cannot have a defined derivative at $r = R_0$ but has different left- and right-derivatives. That could entail a problem for the wavefunction at $r = R_0$. Nevertheless, we can suppose that the wavefunction is in fact defined with an infinitesimal smoothing centered at R_0. This introduces a negligible perturbation, but restores the derivative at R_0.

An interesting criticism is found in [16] 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. It seems from the result, that 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 transforming the coupled Dirac radial equations into a Whittaker's differential equation. This method and the similar one using Kummer's equation (see Refs. cited in Appendix A.7), although rather technical, are often used since they correspond to a "standard" process leading to the solutions. These are confluent hypergeometric series (Appendix A.7) as factors of the same exponential functions corresponding to the ansätze taken in the solution indicated in Appendix A.7, in particular the function ρ^s. Of course, with the finite size of the nucleus, there is no longer any divergence at $\rho = 0$ for this exponential. Nevertheless, if considering both the regular and the anomalous solutions at the same time, a complication appears for the convergence of the series when $\rho \to +\infty$: 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 be exactly balanced, when using asymptotic forms of the series. We have to note that the computed coefficients contain the energy parameter E, because of the initial dimensionless transformation of the Dirac radial equations. With these conditions, the authors have to unify the parameter E when they verify the continuity conditions at $r = R_0$. This leads [19, p.2180] to an equation with a single unknown E (in fact they use a dimensionless unknown $E' = E/mc^2$). Here we can see that, if using the solution method proposed in [4] or in [21], then the convergence of the series involved by the ansätze is independent of the crossroad parameter s and that greatly simplifies the problem.

The criticism of the authors [16], 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. We can understand this criticism insofar as the method of the authors has for a goal to increase the precision of the atomic electron energy levels values. 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 of the wavefunction 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 near the nucleus. 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 [17], 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 [9,18], 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. The author shows that, doing this, the modified radial Dirac operator written in matrix form has an additional term not diagonal $\mu_a \frac{\alpha}{r^2}$ in natural units, where $\mu_a = 0.00058$ determines the anomalous magnetic moment of the electron. This matrix of the modified radial Dirac operator is the following:

$$D_r = \begin{pmatrix} mc^2 + V(r) & \hbar c \left(-\frac{\mathrm{d}}{\mathrm{d}r} + \frac{k}{r} \right) - \mu_a V'(r) \\ \hbar c \left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{k}{r} \right) - \mu_a V'(r) & -mc^2 + V(r) \end{pmatrix}. \tag{5}$$

We cite the author: " this term acts as a repulsive interaction that forces the wavefunction away from the singularity ". In fact, the factor is extremely small, but 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 the criticism analyzed in Sections 2.1–2.3 and also to the criticism of [16].

4. Conclusion, Open Questions, and Future Work

In the first part of this paper, we discussed the principal arguments against the deep orbits (DDL) for H atom and we showed how it is possible to resolve the questions raised. Next we analyzed the computational results of [2,14] 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 (or the radial number, since it has the same value) increases. This result seems to indicate that the mean radius of the DDL orbits decreases when n' increases. Though it is not explicitly said 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.

We also noted that another infinite subset of solutions, what we call "pseudo-regular" energy levels, 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. Moreover, we think that the situation of the DDL orbits in an extreme field implies a big strengthening of the several "special" known effects that affect the regular orbits, such as 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 are also predicted by the relativistic-Schrödinger (Klein–Gordon) equation, which does not include spin effects; therefore, this contribution must be limited to the Dirac equations. While the relativistic-Schrödinger equation does not include spin effects and the predicted 'angular momentum' quantum numbers are for quantities that are two orders-of-magnitude lower than the values associated with the Planck constant, we might suggest that there is a 'hidden' variable within quantum mechanics that may be associated with relativity. 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.

Finally, 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 ∞. An alternative to this computation could be to take into account the anomalous magnetic moment of the electron with unmodified Coulomb potential, as mentioned just above. These questions will be the object of further work.

Appendix A. Some Important Points about 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. As it is copiously handled in the literature, we only recall some essential features. We use a minimal formalism, so we do not use tensor notation that would require explanations not useful for the subject of this paper. Likewise we do not call for advanced algebraic knowledge, such as the Clifford Algebra [19] often used in this field. Among the documents that we used, we can cite, in a non-exhaustive way: [4,18,20–24].

A.1. Elements of Genesis of the Dirac Equation

In order to obtain a quantum evolution equation of first order time derivative, and as quantization requires to replace the energy by the time derivative, Dirac first linearized the classical relativistic energy–momentum relation. So, $E^2 = \mathbf{p}^2 c^2 + m^2 c^4$ was replaced by $E = c\boldsymbol{\alpha} \cdot \mathbf{p} + \beta mc^2$, where $\boldsymbol{\alpha}$ denotes a formal vector constituted from three parameters $\alpha_1, \alpha_2, \alpha_3$ and β is a fourth parameter sometimes denoted by α_0. For the quadratic expression of E be fulfilled, α_i and β must verify algebraic relations, in particular $\{\alpha_\mu, \alpha_\nu\} = \alpha_\mu \alpha_\nu + \alpha_\nu \alpha_\mu = 2\delta_{\mu\nu}$ for $\mu, \nu = 0, 1, 2, 3$. One shows that α_i and β must be at least 4×4 matrices and this dimension is sufficient; but several solutions are possible. In standard representation, the *Dirac matrices*, which are Hermitian operators, are defined by:

$$\alpha_i = \begin{pmatrix} \mathbf{0} & \sigma_i \\ \sigma_i & \mathbf{0} \end{pmatrix} \qquad \text{for } i = 1, 2, 3, \text{ and } \quad \beta = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix},$$

where the four components are 2×2 matrices, the σ_i are the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Other representations [18,20] can be used, such as the Majorana or the Weyl (or chiral) matrices.

Next, the linear energy equation was quantized into the "free" Dirac equation in usual way:

$$i\hbar \partial_t \boldsymbol{\psi}(t, \mathbf{x}) = \mathbf{H}_0 \boldsymbol{\psi}(t, \mathbf{x}), \tag{A.1}$$

where the free Hamiltonian $\mathbf{H}_0$, representing the energy of a free particle including the rest-mass energy mc^2 (the right side of the linear energy equation), is the following matrix-valued differential expression:

$$\mathbf{H}_0 = -i\hbar c\, \alpha \cdot \nabla + \beta mc^2. \tag{A.2}$$

So, the Dirac equation can be written in the form of the following wave equation:

$$(i\hbar \partial_t + i\hbar c\, \alpha \cdot \nabla - \beta mc^2)\, \boldsymbol{\psi}(t, \mathbf{x}) = 0. \tag{A.3}$$

By multiplying this equation on the left by $\boldsymbol{\psi}^\dagger$ and its Hermitian adjoint equation on the right by $\boldsymbol{\psi}$, then subtracting, one obtain [4] a conservation equation $\partial_t\rho + \nabla.\mathbf{J} = 0$, where $\rho = \boldsymbol{\psi}^\dagger\boldsymbol{\psi}$ and $\mathbf{J} = c\boldsymbol{\psi}^\dagger\boldsymbol{\alpha}\boldsymbol{\psi}$ are real quantities and ρ, being non-negative, can be interpreted as a position density probability. This is due to the fact that the Dirac equation contains only a first order derivative in time.

In order to match the dimension of the Dirac matrices, the wavefunction $\boldsymbol{\psi}$ has to be a vector-valued function having four complex components. It is called a *spinor* as it can describe the state of a particle with spin $1/2$. One usually regroups the four components of $\boldsymbol{\psi}$ into two 2-vectors: $\boldsymbol{\psi}_a$ with components ψ_1, ψ_2 and $\boldsymbol{\psi}_b$ with components ψ_3, ψ_4.

A.2. Free-particle Solution

Solving the Dirac equation for a free particle highlights very particular features of the solutions, leading to a historical prediction, before the actual discovery, about the existence of "anti-particles". The Dirac equation is equivalent to four simultaneous first-order partial differential equations. They are linear and homogeneous in the components of the spinor $\boldsymbol{\psi}$ formed by the two vectors $\boldsymbol{\psi}_a$ and $\boldsymbol{\psi}_b$. It is natural to try solutions in the forms of plane waves, i.e.

$$\boldsymbol{\psi}_j(r, t) = \mathbf{u}_j e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \qquad \text{for } j = a, b,$$

where the $\mathbf{u}_j$ are two vectors of dimension two. These are eigenfunctions of the energy operator $i\hbar\partial_t$ and of the momentum operator $-i\hbar\nabla$, whose respective eigenvalues are $E = \hbar\omega$ and the vector $\mathbf{p} = \hbar\mathbf{k}$. By developing the Dirac equation, we obtain the following coupled linear equations on the vectors $\mathbf{u}_j$

$$(E - mc^2)\mathbf{u}_a - c(\boldsymbol{\sigma} \cdot \mathbf{p})\mathbf{u}_b = 0,$$

$$(E + mc^2)\mathbf{u}_b - c(\boldsymbol{\sigma} \cdot \mathbf{p})\mathbf{u}_a = 0, \qquad\qquad (A.4)$$

where $\boldsymbol{\sigma}$ denotes the formal vector of the three Pauli matrices and $\boldsymbol{\sigma} \cdot \mathbf{p} = \sigma_1 p_1 + \sigma_2 p_2 + \sigma_3 p_3$. From the coupled equations, we can deduce the relation

$$\mathbf{u}_a = \frac{c^2\mathbf{p}^2}{E^2 - (mc^2)^2}\mathbf{u}_a, \qquad\qquad (A.5)$$

thus the values of the energy E and the momentum $\mathbf{p}$ satisfy the relativistic relation $E^2 = \mathbf{p}^2 c^2 + m^2 c^4$. But for E, we have the choice between the positive square root E_+ and the negative one E_-.

While solving the system of linear equations for the positive energy, we obtain two linear independent solutions by setting a vector ξ with two possibilities

$$\xi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \xi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Then, for each value of $\mathbf{p}$, we have two positive energy solutions that are orthogonal and can be normalized:

$$\mathbf{u} = N_+ \begin{pmatrix} \xi \\ \frac{c(\boldsymbol{\sigma}\cdot\mathbf{p})}{E_+ + mc^2}\xi \end{pmatrix}, \qquad\qquad (A.6)$$

where N_+ is a normalizing factor depending on E_+. We follow the same process for the "negative" energy E_- by taking the previous ansatz with the opposite sign for the exponent, i.e. $i(-\mathbf{k}.\mathbf{r} + \omega t)$, and we can obtain two negative

energy solutions, orthogonal and normalized by a similar factor N_-, obtained by replacing E_+ by E_- in N_+:

$$\mathbf{v} = N_- \begin{pmatrix} \frac{c(\boldsymbol{\sigma} \cdot \mathbf{p})}{E_- - mc^2} \xi \\ \\ \xi \end{pmatrix} \tag{A.7}$$

For both solutions $\mathbf{u}$, the upper components dominate in the non-relativistic case, i.e. if $|\mathbf{p}| \ll mc$ so one names these components the "great components." For the solutions $\mathbf{v}$, it is the opposite situation, i.e. the lower components dominate.

So, the spectrum of the free Dirac operator $\mathbf{H}_0$ is composed of two infinite intervals separated by a gap: $(-\infty - mc^2] \cup [mc^2 + \infty)$. Now the existence of negative energies has to be interpreted. Paul Dirac suggested a "negative-energy sea" filled with electrons, the "Dirac sea", and it would be possible for high-energy photons to promote electrons out of the sea into positive energies where it would be observable; the "hole" left in the sea would be an observable, as a electron but with a positive charge. So he predicted the existence of the positron, the "anti-particle" of the electron, which was discovered later by Carl Anderson [25]. The concept of Dirac sea is no longer used, particularly in the context of the "single particle" interpretation of the Dirac equation, where it entails some difficulties. Instead and as the relativistic context needs to consider states with unspecified number of particles, QFT [5,20] uses Fock spaces with "2^d quantization", i.e. creation/annihilation operators, particles number operator, etc… But one can see a reminiscence of the Dirac sea in the QED concept of "vacuum polarization."

A.3. Covariance of the Dirac Equation, Spin 1/2

As the Dirac equation was built for being compatible with relativistic effects, it has to be invariant under changes of Lorentz frames. First one can give the Dirac equation a more relativistic form, by multiplying the initial Dirac matrices by the matrix β becoming γ_0, and defining $\gamma_i = \beta\alpha_i$ for $i = 1, 2, 3$. To avoid tensor notation, we use as in [18] the formal notation for bilinear form such as $\langle \gamma, x \rangle := c\gamma_0 t - \gamma \cdot \mathbf{x}$ for any four-vector x in Minkowski space. This form gives a 4×4 matrix and $\gamma.\mathbf{x}$ is the formal scalar product of the spatial vector $\mathbf{x}$ with the vector γ of matrix components γ_i for $i = 1, 2, 3$. Doing this, one can write the Dirac equation in a more symmetric form in space-time variables: $(i\hbar c < \gamma, \partial > -mc^2)\psi = 0$, where ∂ denotes the four-dimensional gradient operator, i.e. a four-vector of differential operators $\partial_0 = {}^1/_c\partial_t$, $\partial_1 = -\partial_x$, $\partial_2 = -\partial_y$, $\partial_3 = -\partial_z$. But beyond the notation, the more important point is that the Dirac equation for a free particle is invariant under the proper orthochronous Poincaré transformations of the space-time coordinates and so it is Lorentz-invariant. Note that the group of general Poincaré transformations is extended to translations in space-time.

We only summarize the relativistic invariance for changes of inertial frames. The corresponding transformations are implemented as unitary operators in the Dirac Hilbert space and they have the following general structure: $\psi(x) \rightarrow \phi(x) = M\psi(\Lambda^{-1}(x-a))$, where Λ is the well-known matrix associated with Lorentz transformations, and M is a linear operator depending on Λ. Here x is a 4-point in Minkowski space, $x = (ct, \mathbf{x})$ and a is associated with a space-time translation. One can show that, when $\psi(x)$ is a solution of the free Dirac equation, $\phi(x)$ is also a solution.

As $(\text{Det } \Lambda)^2 = 1$, we can have $\text{Det}(\Lambda) = \pm 1$. A transformation is *proper* when $\text{Det}(\Lambda) = +1$, i.e. it conserves the direction of the three-space axis of the frame. Moreover the "pure temporal" component Λ^0_0 always satisfies $(\Lambda^0_0)^2 \geq 1$, but the transformation is *orthochronous* only for $\Lambda^0_0 \geq 1$ and, in this case, it conserves the direction of the time axis. For example, the mirror inversion P is improper, but orthochronous, while the time reversal T is also improper, but it is not orthochronous. One can show any proper orthochronous (p.o.) Lorentz transformation is continuously connected to the Identity transformation (which is of course p.o.). This means it can be formed by consecutive infinitesimal transformations starting from the Identity. Moreover, there are two particular classes of p.o. transformations, *boosts*

and *rotations*, and any Lorentz transformation can be written in a unique way as the composition of a boost and a rotation.

Now we note an interesting result justifying the name "spinor": Consider a rotation of angle φ about e.g. the axis of the coordinate x^3. One can show, from the corresponding Lorentz transformation Λ and the operator-associated M, that such a rotation corresponds to application of the matrix

$$\mathbf{M}[\varphi] = \begin{pmatrix} \mathrm{e}^{i\varphi\sigma_3/2} & \mathbf{0} \\ \mathbf{0} & \mathrm{e}^{i\varphi\sigma_3/2} \end{pmatrix}$$

to the spinor $\boldsymbol{\psi}$. As $\mathrm{e}^{i\varphi\sigma_3/2} = \mathrm{I}_2\cos(\varphi/2) + \sigma_3 i\sin(\varphi/2)$, a rotation of angle $\varphi = 2\pi$ gives $\mathrm{M}[2\pi] = -\mathrm{I}_4$ so $\boldsymbol{\psi}$ is transformed into $-\boldsymbol{\psi}$ and we need a rotation of $\varphi = 4\pi$ to obtain the identity transformation. We recognize that a rotation acts on the *spinor* like it does on a particle of *spin* $^1/_2$. So one can see the explanation of spin as a consequence of the union of special relativity and quantum mechanics.

One can find explicit and concise algebraic computations concerning these questions in [20], where the author starts from the matrices γ in the Weyl representation, uses tensor representations and elements of Clifford Algebra [26]. Here is a very elegant tensor form of the free Dirac equation with the matrices γ:

$$(i\gamma^\mu\partial_\mu - m)\boldsymbol{\psi} = 0 \quad \text{where} \ \left(\gamma^0\right)^2 = 1, \ \left(\gamma^i\right)^2 = -1 \text{ for } i \neq 0 \text{ and } \gamma^\mu\gamma^\upsilon = -\gamma^\upsilon\gamma^\mu \quad \text{if } \mu \neq \upsilon.$$

Finally, concerning discrete transformations, we can note that the *CPT* transformation, a combination of the Charge Conjugation, Parity and Time Reversal transformations has for net effect on a free electron wavefunction to convert it into the positron wavefunction. This *CPT* transformation is of a capital importance in Quantum Field Theory [5] because it reverses the up and down two-component spinors in the Dirac wavefunction in the same way as the matrix $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3$

A.4. The Dirac Equation for an Electron in a Coulomb Central Field. The Spin-orbit Operator K Associated with Spin Precession

We consider an electron subjected to an external electromagnetic field, in the form of the static Coulomb potential generated by a proton. Then the vector potential $\mathbf{A}$ can be set to 0, and the scalar potential φ is spherically symmetric. So we have to add the potential energy

$$V = -\frac{e^2}{r} = -\alpha\frac{c\hbar}{r}$$

to the free Hamiltonian $\mathbf{H}_0$, to obtain the "total" Hamiltonian $\mathbf{H} = \mathbf{H}_0 + V\mathbf{I}_4$, where $\mathbf{I}_4$ is the 4D identity matrix.

In principle, the orbital angular momentum $\mathbf{L} = \mathbf{x} \times \mathbf{p}$ commutes with any spherically symmetric function, but it is not a constant of motion in the Coulomb central field as it does not commute with $\mathbf{H}$. One has to add the operator $\mathbf{S} = \frac{1}{4}\hbar\alpha \times \alpha$ where "$\times$" is the formal cross product applied, and α the formal 3-vector of the Dirac matrices $\alpha_1, \alpha_2, \alpha_3$. Then the total angular moment $\mathbf{J} = \mathbf{L} + \mathbf{S}$ is a constant of motion. $\mathbf{S}$ is the *spin operator* of the electron. It is a 3-vector of and its components $\mathbf{S}_i$, for $i = 1,2,3$, are 4×4 matrices. In the standard representation we have

$$\mathbf{S}_i = \frac{1}{2}\hbar\begin{pmatrix} \sigma_i & \mathbf{0}_2 \\ \mathbf{0}_2 & \sigma_i \end{pmatrix}.$$

We can see that $\mathbf{S}$ is a straightforward extension of the usual spin operator $\mathbf{s} = \frac{1}{2}\hbar\sigma$ of the non-relativistic quantum mechanics.

On account of the spherical symmetry of the Coulomb field, one usually uses spherical coordinates to represent the Dirac operator $\mathbf{H}$. So, one can show that the spatial term $\boldsymbol{\alpha} \cdot \mathbf{p}$ of $\mathbf{H}_0$ is transformed into

$$\boldsymbol{\alpha} \cdot \mathbf{p} = \frac{1}{r}(\boldsymbol{\alpha} \cdot \mathbf{x}) \left(p_r + \frac{i\hbar}{r} \beta K \right), \tag{A.8}$$

where p_r is the "radial" momentum given by

$$p_r = \frac{1}{r}(\mathbf{x}.\mathbf{p} - i\hbar) = -i\hbar \left(\partial_r + \frac{1}{r} \right) \tag{A.9}$$

and K is the operator defined by the formula

$$\hbar K = \beta(\boldsymbol{\sigma}' \cdot \mathbf{L} + \hbar), \quad \text{where} \quad \boldsymbol{\sigma}' = \frac{1}{\hbar} 2\mathbf{S} = \begin{pmatrix} \sigma & \mathbf{0}_2 \\ \mathbf{0}_2 & \sigma \end{pmatrix}. \tag{A.10}$$

Here $\mathbf{x}$ represents the vector of the Cartesian coordinates and $r = |\mathbf{x}|$ its norm. The second expression of the radial momentum is its formulation as differential operator in spherical coordinates. Moreover, by substituting the expression of $\boldsymbol{\alpha} \cdot \mathbf{p}$ in $\mathbf{H}$, the "spherical" Hamiltonian now reads:

$$\mathbf{H}_{\text{sph}} = \frac{i\hbar}{r}(\boldsymbol{\alpha} \cdot \mathbf{X}) \left(\partial_r + \frac{1}{r} - \frac{i\hbar}{r} \beta K \right) + \beta mc^2 + V. \tag{A.11}$$

We can see that K is related to the *spin-orbit* term (see Appendix A.5 the relativistic-correction terms).

Moreover one can show that K commutes with the Hamiltonian and it is related to the total angular momentum $\mathbf{J}$ by the relation $\hbar^2 K^2 = \mathbf{J}^2 + \frac{1}{4}\hbar^2$. This expression is obtained by starting from the square of the definition of K. As $\mathbf{J}^2$ has eigenvalues $j(j+1)\hbar^2$, where j can take values $1/2, 3/2, 5/2, \dots$ the Dirac operator defines a *specific quantum number k* for the eigenvalues of the operator K, taking values $\pm 1, \pm 2, \dots$ In fact $k = \mp \left(j \pm \frac{1}{2} \right)$, but it cannot be equal to 0 (see the relation on the square of K). If the quantum number l of $\mathbf{L}$ is j-$1/2$, then the spin (of magnitude $1/2$) and the orbital angular momentum are parallel, else they are anti-parallel. We can say the quantum number k is associated with the spin-orbit interaction. The physical effect of this interaction is the *precession of the electron spin* ([4, p.433,27]).

A.5. The Relativistic Correction Terms Involved by the Dirac Operator. Fine Structure

It is interesting to see what terms are added by the Dirac equation to a non-relativistic Hamiltonian for the electron in a central potential, such as the classical Schrödinger Hamiltonian. For doing this, one can look for a non-relativistic limit of the Dirac equation and then deduce the relativistic perturbations involved in the Dirac operator. This leads first, for the first order correction in v/c, to the 2-components Pauli equation. Next, various and complex methods can be used, such as the Foldy–Wouthyusen transformation [28], to obtain relativistic corrective terms of higher orders in powers of v/c. Supersymmetry techniques can also be used [9,18]. Then one obtains a Hamiltonian $\mathbf{H'}$ with corrections at order $(v/c)^2$ having the following form:

$$\mathbf{H}' = mc^2 + \frac{\mathbf{p}^2}{2m} + V - \frac{\mathbf{p}^4}{8m^3c^2} + \frac{\hbar}{4m^2c^2} \frac{1}{r} \frac{dV}{dr} \boldsymbol{\sigma} \cdot \mathbf{L} + \frac{\hbar^2}{8m^2c^2} \Delta V. \tag{A.12}$$

– In this expression, we first recognize the rest mass energy added to the non-relativistic Hamiltonian, i.e. the non-relativistic kinetic energy plus the potential energy.

– The next (second) term corresponds to a relativistic kinetic energy correction. It can be obtained by expanding $E - mc^2$, where E is the relativistic energy defined by $E^2 = \mathbf{p}^2 c^2 + m^2 c^4$.

– The third term corresponds to the *spin-orbit* energy, interaction energy between the spin $\boldsymbol{\sigma}$ and the orbital movement $\mathbf{L}$ of the electron. One can physically explain this interaction by the fact that, even in a "pure" electrostatic field, the electron moving in this electric field can also "see" a magnetic field. As the electron has a magnetic moment due to its spin, the magnetic field causes a spin precession (Larmor precession), but this would give twice the spin-orbit term. In fact it is half compensated by an extra relativistic effect on the accelerated frame of the electron, causing an additional spin precession with opposite sign, the *Thomas precession* (for a simple derivation, see [29]). We note that the electron is assumed to be slightly relativistic, so the angular velocity ω_T of the Thomas precession is computed by making a first-order approximation to the coefficient $\gamma = \frac{1}{\sqrt{(1-\beta^2)}} \approx 1 + \frac{1}{2}\beta^2$. Then one usually takes for a velocity v, $\omega_T \approx (1/2c^2)\,\dot{\mathbf{V}} \times \mathbf{V}$, while Larmor precession is $\omega_L = -(1/c^2)\,\dot{\mathbf{V}} \times \mathbf{V} = -2\omega_T$.

– Finally the fourth term, called *Darwin term*, is another relativistic correction, but it does not involve angular momentum. This term begins at the non-relativistic limit where the electron is not like a point charge but as a distribution of charge and current in a domain of linear dimension $\hbar/mc$. Physically, it is generally related to the *Zitterbewegung*, a rapid quantum oscillations of the electron blurring the electrostatic interaction with the nucleus and affecting only the s-orbits. Moreover, there is an apparent paradox concerning the spectrum of the standard velocity operator for the position operator, which would consist of $\pm c$. This paradox can be removed by projecting the velocity operator to the particle and the anti-particle sub-spaces of the Hilbert space of the Dirac operator (see e.g. [30]). Quantum Electrodynamics can interpret the Zitterbewegung as quantum fluctuations that allow the creation of particle-antiparticle pairs yielding perturbations of the electric potential [24]. Sometimes one considers it is caused by interference between positive- and negative-energy components [18,31]. Nevertheless, there are also alternative explanations, such as in [32].

Note that the relativistic corrective terms provide an explanation to the physical observation of the fine structure of the Hydrogen and alkali atoms [33]. In fact these effects are not all additive, so the global spin-orbit interaction lowers the effect of the relativistic kinetic energy correction and improves the precision of the corresponding energy w.r.t. measured values. That is an improvement in comparison with the Klein–Gordon equation, which includes also a term of relativistic mass correction and even a Zitterbewegung effect, but no spin-orbit interaction. Nevertheless, the Dirac equation does not account for still subtler spectroscopic observations. It is the case for the hyperfine structure, due to (nucleus) spin-(electron) spin interaction not included in the Dirac Hamiltonian, because the proton is represented only by its Coulomb potential. And also for the Lamb shift, explained in principle by QED effects such as self-energy and vacuum polarization.

Finally, we note that the transformations leading to **H'** are usually done under the hypothesis $E - mc^2 \ll mc^2$ and $|V| \ll mc^2$, what is the case for atomic electrons of hydrogen. However, if the electron is at small distances from the nucleus, therefore in *a very strong electric field* (e.g. for heavy atoms with Z near $1/\alpha$ or for electrons in deep Dirac levels), one should take into account an additional non-linear attractive term of the form $-V^2/2mc^2$ [4,34,35].

A.6. Separation of the Radial Equation

As we consider the case of an electron in a Coulomb central potential, we first use the fact that the potential is time-invariant. So we can separate the time factor from the wavefunction and write $\boldsymbol{\psi}\,[E, \mathbf{x}, t] = \boldsymbol{\psi}(E, \mathbf{x})\,\mathrm{e}^{(-iEt/\hbar)}$, where we explicitly indicate that the eigenfunction $\boldsymbol{\psi}$ does depend on an eigenvalue E of the Hamiltonian **H**. This leads to the stationary equation $\mathbf{H}\boldsymbol{\psi}(E, \mathbf{x}) = E\boldsymbol{\psi}(E, \mathbf{x})$. Here, $\mathbf{x}$ represents the vector of the Cartesian spatial coordinates.

Next, the stationary equation can be separated in spherical coordinates in a similar, but more complex, manner than in the case of the Schrödinger equation for at least two reasons: in the Dirac theory, the wavefunctions are 4-D, and the

angular momenta are "interlaced" in the four components of the spinors. Here we give only an outline of the required process, which is rather technical and cumbersome. So, in (Appendix A.4) the separation was prepared by defining the radial momentum and the operator K. The following transformed Hamiltonian has been obtained:

$$\mathbf{H}_{\text{sph}} = \frac{i\hbar}{r}(\boldsymbol{\alpha} \cdot \mathbf{x}) \left(\partial_r + \frac{1}{r} - \frac{i\hbar}{r}\beta\text{K} \right) + \beta mc^2 + V. \tag{A.13}$$

As in the classical example of the Schrödinger equation, the separation needs two stages:

(a) first, solve the problem of eigenvalues of the angular operators involved in the equation;

(b) next, look for eigenfunction solutions (of the first problem) satisfying the equation.

(a) One may consider the "usual" angular operators J^2, J_z and the new operator K acting only on the angular coordinates, so the eigenvalue problem is independent of r. Moreover, they commute between them. So there is a system of common orthogonal eigenvectors belonging to the Hilbert space $L^2(S^2)^4$ of the square integrable functions on the sphere S^2, for the operators J^2, J_z and K, with respective associated discrete eigenvalues. This allows one to define couples of 2-D spherical spinors $\boldsymbol{\omega}(\theta, \phi)$ similar to the couples of half-spinors defined at the end of (Appendix A.1) and each can be expressed by means of the classical spherical harmonics, which are eigenfunctions of L^2, L_z, considered as functions of the spherical angles θ and φ. The 2-D spinors $\boldsymbol{\omega}(\theta, \varphi)$ provide eigenfunctions of K, the only angular operator occurring in the spherical Hamiltonian $\mathbf{H}_{\text{sph}}$, with associated eigenvalue k.

(b) Now one considers such "angular" eigenfunctions $\boldsymbol{\omega}(\theta,\varphi)$ to form the eigenfunctions $\boldsymbol{\psi}$ common to $\mathbf{H}_{\text{sph}}$ and K.

A wavefunction $\boldsymbol{\psi}$ solution of the Dirac equation can be expressed by a 2-D vector of two 2-D wavefunctions $\boldsymbol{\psi}_1$, $\boldsymbol{\psi}_2$ of the form $\text{X}(r)\,\boldsymbol{\omega}(\theta, \varphi)$, where $\text{X}(r)$ is a scalar function. Here we do not write the quantum numbers in indices (usually k, m or $k, j\pm1/2$). While substituting into the eigenvalue radial equation derived from $\mathbf{H}_{\text{sph}}\boldsymbol{\psi}(E,\mathbf{x}) = E\boldsymbol{\psi}(E,\mathbf{x})$, the operator K is replaced by its eigenvalue represented by k. We note that, while decomposing the Hamiltonian into two halves, some simplifications arise: $\boldsymbol{\alpha}.\mathbf{x}$ applied to the 2-D vector

$$\boldsymbol{\psi} = \begin{pmatrix} \boldsymbol{\psi}_1 \\ \boldsymbol{\psi}_2 \end{pmatrix}$$

is reduced to $\boldsymbol{\sigma}' \cdot \mathbf{x}$ applied to

$$\begin{pmatrix} \boldsymbol{\psi}_2 \\ \boldsymbol{\psi}_1 \end{pmatrix} \quad \text{that gives} \quad \begin{pmatrix} (\boldsymbol{\sigma}\cdot\mathbf{x})\boldsymbol{\psi}_2 \\ (\boldsymbol{\sigma}\cdot\mathbf{x}.)\boldsymbol{\psi}_1 \end{pmatrix}.$$

Next the pseudo-vector nature of $\boldsymbol{\sigma} \cdot \mathbf{x}$ allows us to simplify its application on the spherical spinors, as application of a constant matrix.

A very explicit and detailed process of separation of the radial equation can be found in [21]. From here, and also in the next section (Appendix A.7), we follow the procedure indicated in [4] to obtain and to solve the system of radial equations, because it is technically simple and we can easily see what is done. The radial part $\text{X}(r)$ of the wavefunction $\boldsymbol{\psi}(\mathbf{x})$ solution of the Dirac equation, has two components $F(r)/r$, $G(r)/r$ depending on the radius r and associated with a couple of spherical spinors. Finally, one obtains a system of coupled first order differential equations on the radial functions F and G, valid for any electric central potential with spherical symmetry.

$$\left(E - mc^2 - V \right) F + \hbar c\frac{\text{d}G}{\text{d}r} + \frac{\hbar ck}{r}G = 0,$$

$$\left(E + mc^2 - V\right) G - \hbar c \frac{\mathrm{d}F}{\mathrm{d}r} + \frac{\hbar ck}{r} F = 0. \tag{A.14}$$

Because of the definition of $\boldsymbol{\psi}(\mathbf{x})$ in term of the functions F and G, the required normalization condition on $\boldsymbol{\psi}(\mathbf{x})$ is equivalent to the condition

$$\int_{R+} \left(F^2 + G^2\right) \mathrm{d}r = 1.$$

Different processing of the spherical spinors leads to a different, but very similar, system of coupled equations. In fact, one always recognizes all the same terms, such as $(E - mc^2 - V)$, $(E + mc^2 - V)$, the derivatives of the radial functions, kG/r, etc…, but the signs of the coefficients can change.

A.7. Equation Solution

When considering a Coulomb potential and hydrogen-like atoms, the Coulomb potential energy is equal to $V(r) = -Ze^2/r$ and, in this case, analytical solutions can be obtained. As usual, one defines some parameters that allow the introduction of a dimensionless radius variable and pure numerical equations (we use identifiers different from those in [4] to avoid confusion with the matrices α_i and the coupling constant α):

$$\beta_1 = \frac{mc^2 + E}{\hbar c}, \qquad \beta_2 = \frac{mc^2 - E}{\hbar c}, \qquad \beta = \sqrt{\beta_1 \beta_2}, \qquad \rho = \beta r, \quad \gamma = \frac{Ze^2}{\hbar c}. \tag{A.15}$$

An ansatz is defined in two stages:

(1) First one sets $F(\rho) = f(\rho)\mathrm{e}^{-\rho}$, $G(\rho) = g(\rho)\mathrm{e}^{-\rho}$. Then the equations become

$$g' - g + k\frac{g}{\rho} - \left(\frac{\beta_2}{\beta} - \frac{\gamma}{\rho}\right) f = 0, \tag{A.16a}$$

$$f' - f - k\frac{f}{\rho} - \left(\frac{\beta_1}{\beta} + \frac{\gamma}{\rho}\right) g = 0. \tag{A.16b}$$

(2) Next one looks for solutions in the form of power series, where a_n is the coefficient of the term containing ρ^n:

$$f = \rho^s \left(a_0 + a_1\rho + \cdots\right), \qquad g = \rho^s \left(b_0 + b_1\rho + \cdots\right)$$

with a_0 and $b_0 \neq 0$. While substituting f and g into the coupled equations and after equating the coefficients of ρ^{s+n-1}, one obtains two crossed recurrence relations between the coefficients of the series.

$$(s + n + k) b_n - b_{n-1} + \gamma a_n - \frac{\beta_2}{\beta} a_{n-1} = 0, \qquad (s + n - k) a_n - a_{n-1} - \gamma b_n - \frac{\beta_1}{\beta} b_{n-1} = 0. \tag{A.17}$$

In particular, the relations between a_0 and b_0 are the following, for $n = 0$

$$(s + k) b_0 + \gamma a_0 = 0, \qquad (s - k) b_0 - \gamma a_0 = 0. \tag{A.18}$$

As the determinant of this linear equation system has to be 0, this gives the following condition on s

$$s = \pm\sqrt{\left(k^2 - \gamma^2\right)}. \tag{A.19}$$

Here the choice of the sign plus determines the "regular" solutions, whereas the minus sign leads to the "anomalous" solutions, which are usually rejected. One can obtain a relation between a_n and b_n for any $n > 0$ by multiplying the first of equations (A.18) by β and the second by β_2

$$b_n \left[\beta \left(s + n + k \right) + \beta_2 \gamma \right] = a_n \left[\beta_2 \left(s + n - k \right) - \beta \gamma \right]. \tag{A.20}$$

One can deduce by simple manipulations from relations (A.18), that both series f and g diverge unless, for some integer n', the coefficients a_n and b_n vanish for all $n > n'$.

In these conditions, both equations of (A.18) give the same relation between $a_{n'}$ and $b_{n'}$, i.e. $\beta_2 a_{n'} = -\beta b_{n'}$. Next, by using relation (A.19) and the definitions of the parameters β, β_1 and β_2, we obtain the relation

$$2\beta(s + n') = \gamma(\beta_1 - \beta_2) = \frac{2E\gamma}{\hbar c}, \tag{A.21}$$

where we can remark that the energy E has the sign of the term $(s + n')$. Thus, for $s = +\sqrt{(k^2 - \gamma^2)}$ we have $E > 0$, but if taking $s = -\sqrt{(k^2 - \gamma^2)}$, then $E > 0$ iff $n' > \sqrt{(k^2 - \gamma^2)}$.

From the previous relation, one can obtain the following expression of the energy as functions of the quantum numbers k and n':

$$E = mc^2 \left[1 + \frac{\alpha^2}{\left(n' \pm \sqrt{\left(k^2 - Z^2\alpha^2\right)} \right)^2} \right]^{-1/2}. \tag{A.22}$$

The number n' is the "radial" quantum number and the number $n = n' + |k|$ is the total quantum number. The specific Dirac quantum number k, related to the total angular momentum and corresponding to the physical effect of the spin precession is an important element.

Usually, the regular solutions for the energy level are obtained by taking the positive root for the parameter s in the expression of E, i.e. taking the positive sign between n' and the square root. The choice of $s > 0$ is made for satisfying the boundary conditions at the origin for F and G, $F(0) = G(0) = 0$.

There exist other methods of processing of the initial system of first-order differential equations to obtain the expression of the energy levels E. For example, eliminating one of the two functions of this initial system can lead to a second-order differential equation on the remaining function, such as a Kummer's equation [36]. The solution of this equation is a confluent hypergeometric series $_1F_1$, the coefficients of which are determined to obtain their convergence by reducing them to polynomials ([37], p.7). This method is similar to the one used to solve the Schrödinger equation for the H atom. Other methods can lead to a Whittaker's equation [12,38], a modified form of confluent hypergeometric equations [13].

A.8. Evaluated Equation Solution

A computer program was written by Maly and Va'vra [14] that calculates atomic energy levels for Relativistic Schrodinger levels E1S(+), E2S(−) in Table 1, Dirac levels ED1(+) and ED2(−) in Table 2, and the non-relativistic Schrodinger levels $E(N, Z)$ given by a simple Bohr formula. (Tables from [14] are reprinted here with permission. Copyright November 1993 by the American Nuclear Society, La Grange Park, IL.) Note the lack of a 1s level in the deep levels of Table 2.

Table 1. Relativistic Schroedinger levels for H ($Z = 1$) in eV

	$E(N, Z)$	N	N	L	E1S	E2S
1s	−13.605826	1	0	0	−13.606597	−507171.937500
2p	−3.501457	2	0	1	−3.401449	−13.605632
2s	−3.401457	2	1	0	−3.401570	−13.603699
3d	−1.511759	3	0	2	−1.511747	−3.401425
3p	−1.511759	3	1	1	−1.511755	−509755.250000
3s	−1.511759	3	2	0	−1.511790	−3.401207
4f	−1.511764	4	0	3	−0.850357	−1.511744
4d	−0.850364	4	1	2	−0.850358	−13.605434
4p	−0.850364	4	2	1	−0.850361	−13.604666
4s	−0.850364	4	3	0	−0.850376	−1.511683
5g	−0.850364	5	0	4	−0.544228	−0.850356
5f	−0.544233	5	1	3	−0.544228	−3.401415
5d	−0.544233	5	2	2	−0.544229	−510264.468750
5p	−0.544233	5	3	1	−0.544231	−3.401328
5s	−0.544233	5	4	0	−0.544238	−0.850331
6h	−0.544233	6	0	5	−0.377936	−0.544228
6g	−0.377940	6	1	4	−0.377936	−1.511743
6f	−0.377940	6	2	3	−0.377936	−13.605356
6d	−0.377940	6	3	2	−0.377937	−13.604863
6p	−0.377940	6	4	1	−0.377938	−1.511719
6s	−0.377940	6	5	0	−0.377942	−0.544215

Table 2. Dirac levels of hydrogen-like atoms for H ($Z = 1$) in eV.

	$E(N, Z)$	N	M	K	L1	E1D	L2	E2D	
1s	−13.605826	1	0	1	0	−13.605873	1	−13.605873	*
2p	−3.401457	2	0	2	1	−3.401434	2	−3.401434	*
2s	−3.401457	2	1	1	0	−3.401479	1	−509133.375000	
3d	−1.511759	3	0	3	2	−1.511746	3	−1.511746	*
3p	−1.511759	3	1	2	1	−1.511750	2	−13.605512	*
3s	−0.850364	3	2	1	0	−1.711764	1	−13.604422	
4f	−0.850364	4	0	4	3	−0.850356	4	−0.850356	*
4d	−0.850364	4	1	3	2	−0.850357	3	−3.401419	*
4p	−0.850364	4	2	2	1	−0.850359	2	−510064.125000	
4s	−0.850364	4	3	1	0	−0.850365	1	−3.401298	
5g	−0.544233	5	0	5	4	−0.544228	5	−0.544228	*
5f	−0.544233	5	1	4	3	−0.544228	4	−1.511744	*
5d	−0.544233	5	2	3	2	−0.544229	3	−13.605389	*
5p	−0.544233	5	3	2	1	−0.544230	2	−13.604785	
5s	−0.544233	5	4	1	0	−0.544233	1	−1.511710	
6h	−0.377940	6	0	6	5	−0.377936	6	−0.377936	*
6g	−0.377940	6	1	5	4	−0.377936	5	−0.850356	*
6f	−0.377940	6	2	4	3	−0.377936	4	−3.401412	*
6d	−0.377940	6	3	3	2	−0.377937	3	−510381.343750	
6p	−0.377940	6	4	2	1	−0.377937	2	−3.401344	
6s	−0.377940	6	5	1	0	−0.377939	1	−0.850342	

*Negative energy states, not observable.

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Note Added in Review

The authors wish to thank the reviewer for bringing the topic of Nuclear Collapse [34,35] to our attention. While we had not considered the deep-electron *atomic* orbitals of heavy atoms to be part of our deep-electron story, a quick review of the suggested references indicates both experimental evidence and a theoretical basis for confirming the existence of deep-electron orbits beneath those of the atomic orbitals. The references suggest a desired alternative means of populating the deep-Dirac levels (DDLs), since direct population via photo-emission is so highly forbidden. Furthermore, the relativistic DDL electrons provide an alternative to, or basis for, the reference-proposed dense-electron plasma for initiating collapse to super-heavy nuclei. Exploring both fields together certainly appears to be a desirable pursuit.

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