Original Research Article

A 2D formulation for the helium atom using a four-spinor Dirac-like equation and the discussion of an approximate ground state solution.

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ABSTRACT

We present a two dimensional analysis of the helium atom problem which comes from the classical conservation theorems that allows to use the standard Dirac matrices in order to obtain a four spinor version of the Dirac equation for the two electrons bound problem. Two methods of getting approximated solutions are discussed, although in principle the system of equation can be solved analytically. For one of the methods the separation of the set of equations in its angular and radial parts is made and an approximated solution for the radial system of equations is discussed for the ground state of the atom.

Keywords: [Helium Atom, Dirac Equation, Relativistic Quantum Mechanics, Variational Methods, Hylleraas Method, Semi Analytic Solutions].

1. INTRODUCTION

In this year complete 100 years the two papers of A. Sommerfeld [1] that tried to extend the precarious calculations of the atomic Bohr´s model for the Helium atom to a solid mathematical context through the technique of the action integrals. Unfortunately, it did not work so well as it did in the Hydrogen atom and Quantum Chemistry had to wait more than 10 years, with the arriving of Schroedinger´s Non Relativistic Wave Mechanics and the Hartree-Fock iterative numeric calculations, to become possible reasonably succeeded calculations of the atomic and molecular energies and equilibrium distances for any element of the Periodic Table. However, E. Hylleraas [2] introduced, at the end of the 1920 decade, a new kind of calculation which recovered the variational procedure introduced by Schroedinger and that succeed in the calculation of the ground state energy of the Helium atom. With the advent of the early versions of the Relativistic Quantum Mechanics; the more sophisticated Dirac´s Quantum Theory [3]; the Heisenberg´s creation of the Quantum Electrodynamics at the end of the 1920´s and finally the inclusion of retardation effects in the potential functions [4] made by G. Breit in the beginning of the1930´s, it became possible to take into account the fine structure of the energy levels and to begin to execute highly accurate determinations of the atomic and molecular structures. All of these remarkable developments were well synthesized in the marvellous book of Bether and Salpeter of 1957 [5]. However, Breit´s retardation effects were introduced in a non covariant form and the Hartree-Fock-like iterative calculations are of cumbersome nature, that is, are like a magic box from which the solutions appears as a magical effect. Therefore, the search for a more analytical or understandable structure of calculus, at least in the Hylleraas sense, has been a constant trend in Quantum Chemistry, as are good examples the

Eisenhart´s attempt of making a rigorous analytic separation of variables in the Helium non relativistic Schroedinger equation [6] and the Katos´s investigations [7]. Of course, due to the great manageability and operacionality of the purely computational calculations, they have predominated over more analytical structures in the last decades; despite of this some authors have tried to give an analytical foundation to its iterative calculations, some of which became the inspiration source to start our own work [8,9].

We have since the beginning of our works [10,11] tried to explore the Classical Conservation Theorems *before* any quantization procedure were performed because we believe that they can reduce the dimensions of the coordinate systems which are necessary to formulate the problem in the Quantum domain. More recently, [12] we have shown that it is possible to use 2x2 Dirac matrices associated with a Dirac-like equation instead the usual 4x4 matrices in the analytical solution of the Hydrogen atom which yields a considerable reduction of the complexity of the problem. Besides, our method conducted us to a new formulation of the Hylleraas variational procedure in which the Dirac-like equation is derived from an extremum problem; it is then used to perform numerical calculations that for hydrogenic atoms worked as accurate as we could go in a computational scheme [13].

In the present work, we try to get the same reduction in the dimensions of the Dirac matrices for the problem of the Helium atom, which allows us to use 4x4 matrices instead of the 16x16 matrices of the Breit theory for the Helium atom, which in spite of this is our starting point, although we do not consider the retardation effects in this work. We also obtain the Lagrangean density which is equivalent to the Dirac-like equation for the Helium atom and indicate the calculation structure whose execution will be left for a next paper.

Here we develop a two folded procedure: a first one in which the system is treated as a whole system without a distinction of the particular equations for each electron and a second one in which we use a procedure that preserves the individual identity of each electron. This second procedure takes into account the trivial fact of relativity theory that we can not sum up the geodesics of individual particles. To accomplish this we consider first a single electron plus the nucleus, i.e., the He^+ ion, as the background system into which we introduce the second electron through a penetration parameter which allows the superposition of the individual Hamiltonian equations. This yields a system of differential equations whose wave function is a solution for the whole system, depending on the penetration parameter, which is used at the end of the calculation to obtain the least energy configuration of the system.

For both the procedures we try to express the resulting equations in a truly covariant system of equations in which we can futurely introduce the retardation effects without breaking the covariance requirement.

In the last section of the paper we present [14] a procedure to separate the angular and radial parts of the partial differential equations that come from our Helium Dirac-like equation and found the angular eigenfunctions that allow us to separate the system of radial equations. We then solve the radial equations system asymptotically, from which we get a determination of the ground state energy which agrees within 0.1% with the experimental data and also verify that the exact ion limit is reached when the invader electron goes to infinity.

2. THEORY

In the infinity mass nucleus rest frame, the relativistic classical Hamiltonians for the individual electrons of the Helium atom in natural units $\hbar = c = 1$ and $\alpha = e^2 \cong 1/137$ are

$$H_1 = \sqrt{\mathbf{p}_1^2 + m^2} - \frac{2\alpha}{r_1} + \frac{\alpha}{r_{12}}, \qquad H_2 = \sqrt{\mathbf{p}_2^2 + m^2} - \frac{2\alpha}{r_2} + \frac{\alpha}{r_{12}}, \tag{1a,b}$$

where $r_{12} = \sqrt{r_1^2 + r_2^2 - 2r_1r_2\cos\theta}$. We see that the repulsion energy entries fully for each electron in this case, on the other hand, if we consider the energy of the whole system, not taking into account the electron individualities, we arrive at the usual classical Hamiltonian

$$H = \sqrt{\mathbf{p}_1^2 + m^2} + \sqrt{\mathbf{p}_2^2 + m^2} - \frac{2\alpha}{r_1} - \frac{2\alpha}{r_2} + \frac{\alpha}{r_{12}}, \tag{1c}$$

in which the repulsion energy entries only once.

In the infinity mass nucleus rest frame, we choose to use a coordinate system in which the motion occurs in the plane defined by the nucleus and the two electrons, i.e., $p_z = 0$, whose z axis may be moving at constant velocity with respect to the z axis of another inertial system, so that the system is invariant against space translations in this direction. In this frame, the only non vanishing components of the classical angular momenta of each electron $\mathbf{J}_1 = \mathbf{r}_1 \times \mathbf{p}_1$ and $\mathbf{J}_2 = \mathbf{r}_2 \times \mathbf{p}_2$ and of the total angular momentum $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$ are their z components, namely, $J_{1z} = x_1 p_{1y} - y_1 p_{1x}$, $J_{2z} = x_2 p_{2y} - y_2 p_{2x}$ and $J_z = J_{1z} + J_{2z}$. Now, we know from Classical Mechanics [15] that the Poisson Bracket for each electron angular momentum with respect to the Classical Hamiltonian (1c) is not null and that they are symmetric with respect to each other, i.e., $\{H, J_{1z}\} = r_1 r_2 r_{12}^{-3} \sin\theta = -\{H, J_{2z}\}$, in which $\theta = \theta_2 - \theta_1$, so that its summation is null and hence the total angular momentum J_z becomes a constant of the motion. This happens because the repulsion force between the electrons is a non central force and hence it produces a torque in each electron that makes it oscillating about the axis that join the nucleus to the other electron. In the Poisson Bracket it appears due to the implicit derivatives of $1/r_{12}$ with respect to x_1, y_1 or x_2, y_2, which produces the symmetric terms because $r_{12} = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$ in Cartesian coordinates.

Therefore, a 2D formulation of the problem is, at least in principle, perfectly possible and we shall present two possibilities of it below.

In this way, besides the usual Hamiltonian for the whole system (1c), an alternative approach for the problem would be to define an effective Hamiltonian function for the two electron system which would be composed of a inner Hamitonian H_1 of the ion H_e^+ and an outer Hamiltonian H_2 which would take into account an invader electron, which is superposed to the former through a penetration factor σ, that is

$$H_\sigma = \left(1-\sigma\right) H_1 + 2\sigma H_2 . \tag{1d}$$

We see that $\sigma = 0$ corresponds to the ion limit when $r_{12} \to \infty$ and the electron 2 is not present; on the other hand, $\sigma = 1$ correspond to the limit when the two electrons form a single system with perfectly symmetric positions so that the system Hamiltonian becomes two times the Hamiltonian of one of the electrons, which was chosen by convenience to be the electron 2. In fact, it will be seen that $\rho = \left\langle r_{12} \right\rangle$ will become a function of σ, so that the equations of the system will be solved for r_{12} = constant and then, at the final of the calculation, this constant is varied through σ in order the equilibrium configuration may be obtained.

We now search for a Dirac equation corresponding to the quantization of the classical Eqs. (1c) and (1d), in the infinity nucleus rest frame. The quantization is done in a way similar to that performed by Breit, in which each square root is “linearized” individually:

$$\mathbf{p}_1^2 + m^2 = \left(\gamma^5 p_{1y} - \gamma^3 p_{1x} + m\gamma^0\right)^2 , \tag{2a}$$

$$\mathbf{p}_2^2 + m^2 = \left(\gamma^1 p_{2y} - \gamma^2 p_{2x} + m\gamma^0\right)^2 . \tag{2b}$$

We need five 4×4 anticommuting matrices, which are the four usual γ^μ Dirac matrices together with the γ^5 matrix which always appears connected with Dirac´s theory:

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \boldsymbol{\gamma} = \begin{pmatrix} 0 & \boldsymbol{i\sigma} \\ -\boldsymbol{i\sigma} & 0 \end{pmatrix}, \quad \gamma^5 = -i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{3}$$

where $\sigma_x, \sigma_y, \sigma_z$ are the Pauli spin matrices. As is well known, the γ matrices obey $\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\delta^{\mu\nu}$, for $\mu, \nu = 0,1,2,3,5$, that is, are unitary and anticommute in pairs, as required to make equal the two sides of Eqs.(2).

By using the momenta operators $\mathbf{p}_1 = -i\nabla_1$ and $\mathbf{p}_2 = -i\nabla_2$, the linear Hamiltonian-like matrix operator associated with Eqs.(1c,d) become

$$\hat{H} = i\left(\gamma^3\partial_{x_1} - \gamma^5\partial_{y_1}\right) - \frac{2\alpha}{r_1} + i\left(\gamma^2\partial_{x_2} - \gamma^1\partial_{y_2}\right) - \frac{2\alpha}{r_2} + 2m\gamma^0 + \frac{\alpha}{r_{12}}. \tag{4a}$$

$$\hat{H}_\sigma = (1-\sigma)\left[i\left(\gamma^3\partial_{x_1} - \gamma^5\partial_{y_1}\right) - \frac{2\alpha}{r_1}\right] + 2\sigma\left[i\left(\gamma^2\partial_{x_2} - \gamma^1\partial_{y_2}\right) - \frac{2\alpha}{r_2}\right] + (1+\sigma)\left(m\gamma^0 + \frac{\alpha}{r_{12}}\right). \tag{4b}$$

In our coordinate system the total angular momentum become the z component alone, which in operator form becomes

$$\hat{J}_z = iy_1\partial_{x_1} - ix_1\partial_{y_1} + iy_2\partial_{x_2} - ix_2\partial_{y_2}. \tag{5}$$

But here, due to the non commutativity of the differential operators and matrices in both the Hamiltonians (4) and the total angular momentum (5), the operator $\hat{J}_z$ does not commute with $\hat{H}$, that is, it can be directly shown that $\left[\hat{H}, \hat{J}_z\right] = \gamma^5\partial_{x_1} + \gamma^3\partial_{y_1} + \gamma^2\partial_{x_2} + \gamma^1\partial_{y_2}$, or with $\hat{H}_\sigma$, that is, $\left[\hat{H}_\sigma, \hat{J}_z\right] = (1-\sigma)^2\left(\gamma^5\partial_{x_1} + \gamma^3\partial_{y_1}\right) + 4\sigma^2\left(\gamma^2\partial_{x_2} + \gamma^1\partial_{y_2}\right)$ as well. However, it can be verified that this failure may be immediately compensated by considering a new total angular operator $\hat{M} = \hat{J}_z + \frac{1}{2}\alpha_{1z} + \frac{1}{2}\alpha_{2z}$ for both (4a) and (4b), which assures that $\left[\hat{H}, \hat{M}\right] = 0$ as well as $\left[\hat{H}_\sigma, \hat{M}\right] = 0$. In the definition of this operator were introduced the supplementary anticommutative matrices $\alpha_{1,z} = -i\gamma^5\gamma^3 = \begin{pmatrix} -\sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}$ and $\alpha_{2,z} = -i\gamma^2\gamma^1 = \begin{pmatrix} -\sigma_z & 0 \\ 0 & -\sigma_z \end{pmatrix}$, which cancels the non commutative character of $\hat{J}_z$, so that $\hat{M}$ commutes with both $\hat{H}$ and $\hat{H}_\sigma$. The diagonalization problems to be solved become therefore $\hat{H}\psi = E\psi$ or $\hat{H}_\sigma\psi = E\psi$ and $\hat{M}\psi = j\psi$, where $\psi = (\chi_1, \chi_2, \chi_3, \chi_4)$ is a four-spinor.

Now, in order to get a truly covariant equation, we left-multiply the energy eigenproblem by γ^0, for both operators in (4), so that we get

$$\left[(\phi_{12} - E)\gamma^0 + i\left(\gamma^0\gamma^5\partial_{x_1} - \gamma^0\gamma^3\partial_{y_1}\right) + i\left(\gamma^0\gamma^1\partial_{x_2} - \gamma^0\gamma^2\partial_{y_2}\right) + 2m\right]\psi = 0, \tag{6a}$$

$$\left[(\phi_{12\sigma} - E)\gamma^0 + i(1-\sigma)\left(\gamma^0\gamma^5\partial_{x_1} - \gamma^0\gamma^3\partial_{y_1}\right) + 2i\sigma\left(\gamma^0\gamma^1\partial_{x_2} - \gamma^0\gamma^2\partial_{y_2}\right) + (1+\sigma)m\right]\psi = 0, \tag{6b}$$

where $\phi_{12} = -\frac{2\alpha}{r_1} - \frac{2\alpha}{r_2} + \frac{\alpha}{r_{12}}$ and $\phi_{12\sigma} = -\frac{2(1-\sigma)\alpha}{r_1} - \frac{4\sigma\alpha}{r_2} + \frac{(1+\sigma)\alpha}{r_{12}}$ are the total potential energy functions. It may immediately be seen that Eqs.(6) can be put in the explicit covariant form $\left[\sigma_1\zeta_{1\mu}\pi_1^\mu + \sigma_2\zeta_{2\mu}\pi_2^\mu\right]\psi = 0$, by rewriting them in terms of the matrix operators $\zeta_{1\mu} = \left(1, -\gamma^0\gamma^5, \gamma^0\gamma^3, \gamma^0\right)$, $\zeta_{2\mu} = \left(1, -\gamma^0\gamma^1, \gamma^0\gamma^2, \gamma^0\right)$ and the effective momentum operators

$\hat{\pi}_k^{\mu} = \left(m, -i\partial_{x_k}, -i\partial_{y_k}, -\frac{2\alpha}{r_k} + \frac{\alpha}{\sigma_3 r_{12}} - \frac{E}{2\sigma_k} \right)$, where $k = 1,2$; $\sigma_1 = \sigma_2 = 1$, $\sigma_3 = 2$ for (6a) and $\sigma_1 = 1 - \sigma$, $\sigma_2 = 2\sigma$, $\sigma_3 = 1$ for (6b).

Explicitly, Eq.(6a) becomes the following system of linear partial differential equations

$$q_+\chi_1 - \left(\partial_{x_1} + i\partial_{y_1}\right)\chi_3 + \left(-\partial_{x_2} + i\partial_{y_2}\right)\chi_4 = 0\,, \tag{7a}$$

$$q_+\chi_2 + \left(\partial_{x_1} - i\partial_{y_1}\right)\chi_4 - \left(\partial_{x_2} + i\partial_{y_2}\right)\chi_3 = 0\,, \tag{7b}$$

$$q_-\chi_3 + \left(-\partial_{x_1} + i\partial_{y_1}\right)\chi_1 + \left(-\partial_{x_2} + i\partial_{y_2}\right)\chi_2 = 0\,, \tag{7c}$$

$$q_-\chi_4 + \left(\partial_{x_1} + i\partial_{y_1}\right)\chi_2 - \left(\partial_{x_2} + i\partial_{y_2}\right)\chi_1 = 0\,, \tag{7d}$$

and Eq.(6b) as well becomes

$$q_{\sigma+}\chi_1 - (1-\sigma)\left(\partial_{x_1} + i\partial_{y_1}\right)\chi_3 + 2\sigma\left(-\partial_{x_2} + i\partial_{y_2}\right)\chi_4 = 0\,, \tag{8a}$$

$$q_{\sigma+}\chi_2 + (1-\sigma)\left(\partial_{x_1} - i\partial_{y_1}\right)\chi_4 - 2\sigma\left(\partial_{x_2} + i\partial_{y_2}\right)\chi_3 = 0\,, \tag{8b}$$

$$q_{\sigma-}\chi_3 + (1-\sigma)\left(-\partial_{x_1} + i\partial_{y_1}\right)\chi_1 + 2\sigma\left(-\partial_{x_2} + i\partial_{y_2}\right)\chi_2 = 0\,, \tag{8c}$$

$$q_{\sigma-}\chi_4 + (1-\sigma)\left(\partial_{x_1} + i\partial_{y_1}\right)\chi_2 - 2\sigma\left(\partial_{x_2} + i\partial_{y_2}\right)\chi_1 = 0\,, \tag{8d}$$

in which the new potential functions $q_{\pm} = 2m \pm \left(\phi_{12} - E\right)$ and $q_{\sigma\pm} = (1+\sigma)m \pm \left(\phi_{12\sigma} - E\right)$ were introduced for shortness.

At this point we shall need to split the paper in two parts. In the first one, we shall present a variational version of Eqs.(7) that will allow us to make numerical calculations of the energy eigenvalues in the Hylleraas scheme, as was already done by us with high accuracy in the one electron atoms [13]. But we shall only introduce the problem, which will be treated fully in a next paper. To do this, firstly we solve the last two equations of (7) for χ_3 and χ_4, what yields

$$\chi_3 = \frac{\left(\partial_{x_1} - i\partial_{y_1}\right)\chi_1 + \left(\partial_{x_2} - i\partial_{y_2}\right)\chi_2}{q_-}\,, \qquad \chi_4 = \frac{-\left(\partial_{x_1} + i\partial_{y_1}\right)\chi_2 + \left(\partial_{x_2} + i\partial_{y_2}\right)\chi_1}{q_-}\,, \tag{9}$$

then we substitute them into the first two of (7), left-multiply each one by the complex conjugated vectors χ_1^* and χ_2^* respectively and sum up the resulting equations to form a real quadratic function in $\left(\chi_1, \chi_2\right)$ which defines the following Lagrangean density

$$\begin{aligned} L = & \frac{\left|\partial_{x_1}\chi_1 - i\partial_{y_1}\chi_1\right|^2 + \left|\partial_{x_1}\chi_2 + i\partial_{y_1}\chi_2\right|^2 + \left|\partial_{x_2}\chi_1 + i\partial_{y_2}\chi_1\right|^2 + \left|\partial_{x_2}\chi_2 - i\partial_{y_2}\chi_2\right|^2}{q_-} + q_+\left|\chi_1\right|^2 + \\ & + \Re\left[\frac{(\partial_{x_1}\chi_1^* + i\partial_{y_1}\chi_1^*)(\partial_{x_2}\chi_2 + i\partial_{y_2}\chi_2) - (\partial_{x_2}\chi_1^* + i\partial_{y_2}\chi_1^*)(\partial_{x_1}\chi_2 + i\partial_{y_1}\chi_2)}{q_-}\right] + q_+\left|\chi_2\right|^2 \end{aligned} . \qquad (10)$$

The extremum problem

$$\delta\int L dx_1 dx_2 dy_1 dy_2 = 0 \qquad (11)$$

is then solved, in the same way as done with the hydrogenic atoms, by the requirement that the integral in (11) be stable against small variations of the algebraic forms of $\left(\chi_1, \chi_2\right)$ about the corresponding exact solutions of (7) or some suitable approximation of them:

$$\chi_\ell = \chi_{\ell ap}\sum_{\mu+\nu+\lambda=0}^{N} c_{\ell\mu\nu\lambda} r_1^{\mu} r_2^{\nu} r_{12}^{\lambda} \qquad (12)$$

for $\ell = 1, 2$ in which $\chi_{\ell ap}$ are the approximations for the exact solutions of (7), $c_{\ell\mu\nu\lambda}$ are the variational coefficients corresponding to each function $\chi_{\ell ap}$ and *N* is the least integer necessary to a given order of precision to be reached. The variation becomes thus

$$\frac{\partial}{\partial c_{\ell\mu\nu\lambda}}\int L dx_1 dx_2 dy_1 dy_2\bigg|_{N=0,1,2,...} = 0, \qquad (13)$$

which produces two systems of linear equations in $c_{\ell\mu\nu\lambda}$, whose dimension is fixed by *N*, the determinants of which generates a polynomial function on the atom energy whose solution yields the energy eigenvalues for the atom. It should be remarked that the need to know $\chi_{\ell ap}$ in advance is in fact the great limitation of the Hylleraas methodology because, in practice, only asymptotic solutions are known, so that the use of arbitrary intermediary functions becomes the only way to perform the calculation. It is by this reason that we are proposing below the sigma variation procedure, in which we retain the almost exact form of the one electron solution and perform the variation through a macro parameter that is related to the average values of the radial variables. The Hylleraas-like problem will be reconsidered formally in a next paper.

3. APPROXIMATE GROUND STATE SOLUTION FOR THE SIGMA HAMILTONIAN

Now, considering the second part of the paper, we shall perform the variation through the parameter sigma which allows using one electron solutions to provide an analytical approximation for the solution of the Eqs.(8). Thus, in order to separate the angular part of Eqs.(8), we must first address the angular momentum problem, $\hat{M}\psi = j\psi$, which written in the polar coordinates of the electrons 1 and 2 becomes $\left(\partial_{\theta_1}+\partial_{\theta_2}\right)\chi_k = i\left(j+\lambda_k\right)\chi_k$, where $\lambda_1 = 1$, $\lambda_2 = -1$, $\lambda_3 = \lambda_4 = 0$, are the diagonal values of $-\frac{1}{2}\left(\alpha_{1z}+\alpha_{2z}\right)$ and $j = j_1 + j_2$. In accordance, the most general forms for the solutions of the angular equation are the set of eigenfunctions

$$\chi_k = f_k e^{i\Phi_k}\,,\quad f_k = f_k\left(r_1, r_2, r_{12}\right),\quad k = 1,..,4\,, \tag{14}$$

where the phase functions are

$$\Phi_1 = \left(j_1+\tfrac{1}{2}\right)\theta_1 + \left(j_2+\tfrac{1}{2}\right)\theta_2 + g_1\,,\quad \Phi_2 = \left(j_1-\tfrac{1}{2}\right)\theta_1 + \left(j_2-\tfrac{1}{2}\right)\theta_2 + g_2\,, \tag{15a,b}$$

$$\Phi_3 = \left(j_1-\tfrac{1}{2}\right)\theta_1 + \left(j_2+\tfrac{1}{2}\right)\theta_2 + g_3\,,\quad \Phi_4 = \left(j_1+\tfrac{1}{2}\right)\theta_1 + \left(j_2-\tfrac{1}{2}\right)\theta_2 + g_4\,, \tag{15c,d}$$

with $g_k = g_k\left(r_1, r_2, r_{12}\right)$. Since $r_{12} = r_{12}(r_1, r_2, \theta)$, the dependence of f_k and g_k on r_{12} has evidently no effect on the values of the angular momentum, but this dependence is necessary when considering a complete solution of the problem in the radial variables r_1, r_2, r_{12}.

Formally, the substitution of χ_k in Eq.(8) makes all complex phases and angular variables vanish and yields a new set of linear equations depending only on the radial variables r_1, r_2, r_{12}. To see this we consider the first order derivatives appearing in (8) expressed in the polar system $\left(r_1, r_2, \theta_1, \theta_2\right)$ and considering also the implicit dependence of the Cartesian coordinates in $r_{12} = r_{12}(r_1, r_2, \theta)$, from this we get the following differential operators

$$\partial_{x_1} \pm i\partial_{y_1} = e^{\pm i\theta_1}\left(\partial r_1 \pm \frac{i}{r_1}\partial\theta_1\right) + \frac{r_1 e^{\pm i\theta_1} - r_2 e^{\pm i\theta_2}}{r_{12}}\partial r_{12}\,, \tag{16a}$$

$$\partial_{x_2} \pm i\partial_{y_2} = e^{\pm i\theta_2}\left(\partial r_2 \pm \frac{i}{r_2}\partial\theta_2\right) - \frac{r_1 e^{\pm i\theta_1} - r_2 e^{\pm i\theta_2}}{r_{12}}\partial r_{12}\,. \tag{16b}$$

Substituting the solution (14) together with the operators (16) into (8) and next separating it in their real and imaginary parts would bring two sets of linear partial differential equations in the radial variables r_1, r_2, r_{12} connecting f_k and g_k with their derivatives, whose analytical solution is completely out of hand at the moment.

However, in this work, we shall limit ourselves to search for solutions satisfying the constraint $\rho = \left\langle r_{12}\right\rangle =$ constant, so that in effect we arrive at $f_k = f_k\left(r_1, r_2\right)$ and further assume that $g_k = 0$, which will simplify considerably the resulting equations and also yields the variational relation $\rho = \rho(\sigma)$ that will be used to get the equilibrium configuration of the system. In these circumstances, we arrive at a unique system of equations given by the real part of (8), the imaginary one vanishing identically, that is

$$q_{\sigma+} f_1 - (1-\sigma)\left(\frac{\partial f_3}{\partial r_1} + \frac{j_1 - \frac{1}{2}}{r_1} f_3\right) - 2\sigma\left(\frac{\partial f_4}{\partial r_2} - \frac{j_2 - \frac{1}{2}}{r_2} f_4\right) = 0\,, \tag{17a}$$

$$q_{\sigma+} f_2 + (1-\sigma)\left(\frac{\partial f_4}{\partial r_1} + \frac{j_1 + \frac{1}{2}}{r_1} f_4\right) - 2\sigma\left(\frac{\partial f_3}{\partial r_2} + \frac{j_2 + \frac{1}{2}}{r_2} f_3\right) = 0\,, \tag{17b}$$

$$q_{\sigma-} f_3 - (1-\sigma)\left(\frac{\partial f_1}{\partial r_1} + \frac{j_1 + \frac{1}{2}}{r_1} f_1\right) - 2\sigma\left(\frac{\partial f_2}{\partial r_2} + \frac{j_2 - \frac{1}{2}}{r_2} f_2\right) = 0\,, \tag{17c}$$

$$q_{\sigma-} f_4 + (1-\sigma)\left(\frac{\partial f_2}{\partial r_1} - \frac{j_1 - \frac{1}{2}}{r_1} f_2\right) - 2\sigma\left(\frac{\partial f_1}{\partial r_2} + \frac{j_2 + \frac{1}{2}}{r_2} f_1\right) = 0\,. \tag{17d}$$

Since the limitations described above do not allow us to get general solutions, we shall limit ourselves to get the simplest solution of Eq.(17), valid only for the ground state of the atom:

$$f_k = e^{-\beta_1 r_1 - \beta_2 r_2} \sum_{\mu+\nu=0}^{1} a_{k\mu\nu} r_1^{s_1+\mu} r_2^{s_2+\nu}\,, \qquad k = 1,2,3,4\,, \tag{18}$$

because the approximation made above restricts heavily the possibility of obtaining energy sub-states that depend strongly on power series of higher degrees. The substitution of Eq.(18), together with its first derivatives

$$\partial r_1 f_k = e^{-\beta_1 r_1 - \beta_2 r_2} \sum_{\mu+\nu=0}^{1} a_{k\mu\nu}\left(\frac{s_1+\mu}{r_1} - \beta_1\right) r_1^{s_1+\mu-1} r_2^{s_2+\nu}\,, \qquad k = 1,2,3,4\,, \tag{19a}$$

$$\partial r_2 f_k = e^{-\beta_1 r_1 - \beta_2 r_2} \sum_{\mu+\nu=0}^{1} a_{k\mu\nu}\left(\frac{s_2+\nu}{r_2} - \beta_2\right) r_1^{s_1+\mu} r_2^{s_2+\nu-1}\,, \tag{19b}$$

into the system (17) yields the new set of equations (summation on μ,ν is omitted for shortness):

$$\left[\gamma_{2\rho} - \frac{2\alpha(1-\sigma)}{r_1} - \frac{4\alpha\sigma}{r_2}\right] a_{1\mu\nu} + (1-\sigma)\left(\beta_1 + \frac{j_1 - s_1 - \frac{1}{2}}{r_1}\right) a_{3\mu\nu} + 2\sigma\left(\beta_2 + \frac{j_2 - s_2 - \frac{1}{2}}{r_2}\right) a_{4\mu\nu} = 0$$

(20a)

$$\left[\gamma_{2\rho} - \frac{2\alpha(1-\sigma)}{r_1} - \frac{4\alpha\sigma}{r_2}\right] a_{2\mu\nu} + 2\sigma\left(\beta_2 - \frac{j_2 + s_2 + \frac{1}{2}}{r_2}\right) a_{3\mu\nu} + (1-\sigma)\left(\frac{j_1 + s_1 + \frac{1}{2}}{r_1} - \beta_1\right) a_{4\mu\nu} = 0$$

(20b)

$$\left[\gamma_{1\rho} + \frac{2\alpha(1-\sigma)}{r_1} + \frac{4\alpha\sigma}{r_2}\right] a_{3\mu\nu} + 2\sigma\left(\beta_2 + \frac{j_2 - s_2 - \frac{1}{2}}{r_2}\right) a_{2\mu\nu} + (1-\sigma)\left(\beta_1 - \frac{j_1 + s_1 + \frac{1}{2}}{r_1}\right) a_{1\mu\nu} = 0$$

(20c)

$$\left[\gamma_{1\rho}+\frac{2\alpha(1-\sigma)}{r_1}+\frac{4\alpha\sigma}{r_2}\right]a_{4\mu\nu}-(1-\sigma)\left(\beta_1+\frac{j_1-s_1-\frac{1}{2}}{r_1}\right)a_{2\mu\nu}+2\sigma\left(\beta_2-\frac{j_2+s_2+\frac{1}{2}}{r_2}\right)a_{1\mu\nu}=0 \tag{20d}$$

where $\gamma_{1\rho}=(1+\sigma)m+E-\frac{(1+\sigma)\alpha}{\rho}$ and $\gamma_{2\rho}=(1+\sigma)m-E+\frac{(1+\sigma)\alpha}{\rho}$. Now we start with the determination of the coefficients and parameters by observing that the system of equations formed by each negative power $1/r_1$ and $1/r_2$ must vanish separately in order the coefficients a_{k00} do not vanish:

$$-2\alpha a_{100}+\left(j_1-s_1-\tfrac{1}{2}\right)a_{300}=0\,, \tag{21a}$$

$$-2\alpha a_{200}+\left(j_1+s_1+\tfrac{1}{2}\right)a_{400}=0\,, \tag{21b}$$

$$-\left(j_1+s_1+\tfrac{1}{2}\right)a_{100}+2\alpha a_{300}=0\,, \tag{21c}$$

$$-\left(j_1-s_1-\tfrac{1}{2}\right)a_{200}+2\alpha a_{400}=0\,, \tag{21d}$$

and equally

$$-4\alpha a_{100}+\left(j_2-s_2-\tfrac{1}{2}\right)a_{400}=0\,, \tag{22a}$$

$$-4\alpha a_{200}-\left(j_2+s_2+\tfrac{1}{2}\right)a_{300}=0\,, \tag{22b}$$

$$-\left(j_2+s_2+\tfrac{1}{2}\right)a_{100}+4\alpha a_{400}=0\,, \tag{22c}$$

$$\left(j_2-s_2-\tfrac{1}{2}\right)a_{200}+4\alpha a_{300}=0\,. \tag{22d}$$

For this condition to be fulfilled it is necessary that the determinants of the systems (21) and (22) vanish, from which we get $s_1=-\frac{1}{2}+\sqrt{j_1^2-4\alpha^2}$ and $s_2=-\frac{1}{2}+\sqrt{j_2^2-4\alpha^2}$.

Now get back to the original system (20), assume that $a_{k\mu\nu}=a_{k\nu\mu}$, for $\mu\neq\nu=0,1$, and equate the coefficients of the system of equations for the same powers, from which we get the system of recurrence equations

$$\gamma_{2\rho}a_{100}+(1-\sigma)\beta_1a_{300}+2\sigma\beta_2a_{400}-2\alpha(1+\sigma)a_{110}-(1-\sigma)s_1a_{310}-2\sigma s_2a_{410}=0\,, \tag{23a}$$

$$\gamma_{2\rho}a_{200}+2\sigma\beta_2a_{300}+(1-\sigma)\beta_1a_{400}-2\alpha(1+\sigma)a_{210}-2\sigma s_2a_{310}+(1-\sigma)s_1a_{410}=0\,, \tag{23b}$$

$$(1-\sigma)\beta_1a_{100}+2\sigma\beta_2a_{200}+\gamma_{1\rho}a_{300}+2\alpha(1+\sigma)a_{310}-(1-\sigma)s_1a_{110}-2\sigma s_2a_{210}=0\,, \tag{23c}$$

$$2\sigma\beta_2a_{100}-(1-\sigma)\beta_1a_{200}+\gamma_{1\rho}a_{400}+2\alpha(1+\sigma)a_{410}-2\sigma s_2a_{110}+(1-\sigma)s_1a_{210}=0\,. \tag{23d}$$

In order the series (18) can stop, the part of the coefficients a_{k00} in the recurrence must vanish separately of that of the coefficients $a_{k\mu\nu}$ for $\mu\neq\nu=0,1$, that is

$$\gamma_{2\rho}a_{100}+(1-\sigma)\beta_1a_{300}+2\sigma\beta_2a_{400}=0\,, \tag{25a}$$

$$\gamma_{2\rho}a_{200}+2\sigma\beta_2a_{300}+(1-\sigma)\beta_1a_{400}=0\,, \tag{25b}$$

$$(1-\sigma)\beta_1 a_{100} + 2\sigma\beta_2 a_{200} + \gamma_{1\rho} a_{300} = 0\,, \tag{25c}$$

$$2\sigma\beta_2 a_{100} - (1-\sigma)\beta_1 a_{200} + \gamma_{1\rho} a_{400} = 0\,, \tag{25d}$$

and also

$$-2\alpha(1+\sigma)a_{110} - (1-\sigma)s_1 a_{310} - 2\sigma s_2 a_{410} = 0\,, \tag{26a}$$

$$-2\alpha(1+\sigma)a_{210} - 2\sigma s_2 a_{310} + (1-\sigma)s_1 a_{410} = 0\,, \tag{26b}$$

$$2\alpha(1+\sigma)a_{310} - (1-\sigma)s_1 a_{110} - 2\sigma s_2 a_{210} = 0\,, \tag{26c}$$

$$2\alpha(1+\sigma)a_{410} - 2\sigma s_2 a_{110} + (1-\sigma)s_1 a_{210} = 0\,. \tag{26d}$$

Therefore in order the system (25) have a non trivial solution its determinant must vanish, from what we get $\beta_1 = \frac{\sqrt{\gamma_{1\rho}\gamma_{2\rho} - 4\sigma^2\beta_2^2}}{1-\sigma}$ as a function of β_2 and the other parameters.

Now, the non trivial solution for the homogeneous system of equations (25) in the coefficients a_{k00} can be obtained from the kernel associated to the β_1, whose basis is given by the two linearly independent column vectors

$$\psi_1 = \begin{pmatrix} -(1-\sigma)\beta_1/\gamma_{2\rho} \\ -2\sigma\beta_2/\gamma_{2\rho} \\ 1 \\ 0 \end{pmatrix}, \qquad \psi_2 = \begin{pmatrix} -2\sigma\beta_2/\gamma_{2\rho} \\ -(1-\sigma)\beta_1/\gamma_{2\rho} \\ 0 \\ 1 \end{pmatrix}, \tag{27a,b}$$

out of which $\psi = a_{300}\psi_1 + a_{400}\psi_2$ is a general kernel vector. These basis vectors generate by its turn relations among the power series coefficients given by $a_{100} = -(1-\sigma)\beta_1 a_{300}/\gamma_{2\rho}$, $a_{200} = -2\sigma\beta_2 a_{300}/\gamma_{2\rho}$, $a_{400} = 0$ for the former vector and $a_{100} = -2\sigma\beta_2 a_{400}/\gamma_{2\rho}$, $a_{200} = -(1-\sigma)\beta_1 a_{400}/\gamma_{2\rho}$, $a_{300} = 0$ for the later one.

The last step in order to be able to make the evaluation of the energy eigenvalue of the system is as follows. First form a null line vector corresponding to the system (23), i.e., $R = [23a, 23b, 23c, 23d]$ and second make a contraction of it with one of the kernel vectors. Since it may be seen that both kernel vectors produce the same energy eigenvalue, so that the solutions in a_{300} and a_{400} are degenerated, we choose to make the contraction with the first kernel vector, that is, $R\psi_1 = 0$. This operation, as expected, eliminates the coefficients a_{k00} while it produces a new relation connecting the coefficients a_{k10}:

$$\begin{aligned}&\left[\frac{2\alpha\left(1-\sigma^2\right)\beta_1}{\gamma_{2\rho}}-\left(1-\sigma\right)\left(\frac{3}{2}+s_1+j_1\right)\right]a_{110}+2\sigma\left[\frac{2\alpha\left(1+\sigma\right)\beta_2}{\gamma_{2\rho}}-\frac{3}{2}-s_2+j_2\right]a_{210}+\\&+\left[\left(\frac{3}{2}+s_1-j_1\right)\frac{\left(1-\sigma\right)^2\beta_1}{\gamma_{2\rho}}+4\sigma^2\beta_2\left(\frac{3}{2}+s_2+j_2\right)+2\alpha\left(1+\sigma\right)\right]a_{310}=0\end{aligned} \quad . \tag{28}$$

Third, decrease the indices μ by one step, in order we can obtain another relation for the coefficients a_{k00}, and use the relation given by the kernel vector ψ_1 to eliminate them:

$$\begin{aligned}&-\left[\frac{2\alpha\left(1-\sigma^2\right)\beta_1}{\gamma_{2\rho}}-\left(1-\sigma\right)\left(\frac{1}{2}+s_1+j_1\right)\right]\left(1-\sigma\right)\frac{\beta_1}{\gamma_{2\rho}}-4\sigma^2\left[\frac{2\alpha\left(1+\sigma\right)\beta_2}{\gamma_{2\rho}}-\frac{1}{2}-s_2+j_2\right]\frac{\beta_2}{\gamma_{2\rho}}+\\&+\left(\frac{1}{2}+s_1-j_1\right)\frac{\left(1-\sigma\right)^2\beta_1}{\gamma_{2\rho}}+4\sigma^2\beta_2\left(\frac{1}{2}+s_2+j_2\right)+2\alpha\left(1+\sigma\right)=0.\end{aligned} \tag{29}$$

Before we can follow, we should note that the determinant of the system (26) is not null, so that the only possible solution for (26) is the trivial solution, i.e., $a_{k10}=0$, so that the solution (18) for the differential system of equations reduces to the elementary form

$$f_k=a_{k00}r_1^{s_1}r_2^{s_2}e^{-\beta_1 r_1-\beta_2 r_2}\ , \qquad k=1,2,3,4\ , \tag{30}$$

where we have redefined the coefficients a_{k00} as $a_{100}=-\left(1-\sigma\right)\beta_1/\gamma_{2\rho}$, $a_{200}=-2\sigma\beta_2/\gamma_{2\rho}$, $a_{300}=1$ and $a_{400}=0$.

Now, we write by convenience $\beta_2=h\beta_1$, where *h* is to be determined below. As a consequence, substituting β_1 found above and after a little of algebra, we get from (29)

$$\gamma_{1\rho}\gamma_{2\rho}=\frac{4\alpha^2\left(1+\sigma\right)^2\left[\left(1-\sigma\right)^2+4\sigma^2h^2\right]\left(\gamma_{1\rho}-\gamma_{2\rho}\right)^2}{\left(1-\sigma^2\right)\left(s_1+\frac{1}{2}\right)+4\sigma^2h\left(s_2+\frac{3}{2}\right)}\ , \tag{31}$$

which is the fundamental relation that connects the electron parameters. Next, we substitute into (31) the expressions for $\gamma_{1\rho}$ and $\gamma_{2\rho}$ defined above to get finally an algebraic expression for the energy eigenvalues we are searching for

$$E=\frac{\alpha\left(1+\sigma\right)}{\rho}+\frac{\left(1+\sigma\right)m}{\sqrt{1+\dfrac{4\alpha^2\left(1+\sigma\right)^2\left[\left(1-\sigma\right)^2+4\sigma^2h^2\right]}{\left(1-\sigma^2\right)\left(s_1+\frac{1}{2}\right)+4\sigma^2h\left(s_2+\frac{3}{2}\right)}}}\ . \tag{32}$$

However, this is not yet the final step, since we still need to find out a value for *h* and the connection between σ and ρ, so that we can obtain a numerical evaluation of the atom energy. This is done by considering the values of the radii for which the probability given by the radial function (30) is a maximum, that is, for which the first derivatives (19) vanish. From this come the relations $r_{10}=s_1/\beta_1$ and

$r_{20} = s_2 / \beta_2$ among the most likely orbital radii and the points of maxima of the radial part of the wave function.

Further we assume that $\rho = \langle r_{12} \rangle$ at the equilibrium configuration may be approximated by $\rho = r_{10} + r_{20}$ and also a linear connection $r_{10} = \sigma r_{20}$ between the electron equilibrium radii which assures the contour condition $r_{20} \to \infty$ when $\sigma \to 0$. From these relations we finally get $h = \sigma s_2 / s_1$. At this point we have finally fulfilled all the steps toward getting an expression for the energy eigenvalues in terms of the basic electron properties along with the variation factor σ:

$$E = \frac{2\sigma m\alpha^2 (1+\sigma)^2}{C_1} + \frac{(1+\sigma)m}{C_2}\,, \tag{33}$$

where use has been made of the parameters

$$C_1 = \sqrt{\left[(1-\sigma)^2 (s_1 + \tfrac{1}{2})s_1 + 4\sigma^3 (s_2 + \tfrac{3}{2})s_2\right]^2 + 4\alpha^2 (1+\sigma)^2 \left[(1-\sigma)^2 s_1^2 + 4\sigma^4 s_2^2\right]}\,, \tag{34a}$$

$$C_2 = \sqrt{1 + \frac{4\alpha^2 (1+\sigma)^2 \left[(1-\sigma)^2 s_1^2 + 4\sigma^4 s_2^2\right]}{\left[(1-\sigma)^2 (s_1 + \tfrac{1}{2})s_1 + 4\sigma^3 (s_2 + \tfrac{3}{2})s_2\right]^2}}\,. \tag{34b}$$

We also get, together with Eq.(33), a determination of the equilibrium distance between the electrons as a function of σ, i.e., $\rho = \dfrac{C_1}{2\sigma m\alpha(1+\sigma)}$, as was aimed at the beginning of the paper. And finally the equilibrium radii becomes $r_{10} = \dfrac{\sigma}{1+\sigma}\rho$ and $r_{20} = \dfrac{\rho}{1+\sigma}$.

At this point we can make a plot of the energy excess $\Delta E = E - (1+\sigma)m$ of the system against the effective mass $(1+\sigma)m$. After considering the unit conversion factors, the Hartree $m\alpha^2 \cong 27eV$ and the Bohr radius $a_0 = 1/(m\alpha) \cong 0.53A^{\circ}$, we get dimensionless forms for the energy excess ΔE and for the distance ρ as follows:

$$\Delta E = \frac{2\sigma(1+\sigma)^2}{C_1} + \left[\frac{(1+\sigma)}{C_2} - 1 - \sigma\right]\frac{1}{\alpha^2}\,, \tag{35}$$

$$\rho = \frac{C_1}{2\sigma(1+\sigma)}\,. \tag{36}$$

The plot of the energy excess (in au) as a function of σ is shown in Fig.1, from which we immediately see that the ion ground state limit $\Delta E = -2$ occurs for σ = 0 or $\rho = \infty$. The minimum of the energy excess for $j_1 = j_2 = 1$ corresponds to the inner orbital state of the parahelium atom (or the state 1s-1s of the

Spectroscopy). By solving the equation $\frac{\Delta E}{d\sigma} = 0$, we see that the equilibrium value occurs approximately for $\sigma = 0.17753$, for whose value we get an energy ground state of $\Delta E = -2.9059$, which agrees with the experimental value $\Delta E_{Exp} = -2.9033$ within 0.1% of accuracy. This means that the approximations done to get the determination of the ground state energy of the atom, although rather rough, were consistent with the dynamics of the physical system. Besides, the equilibrium radii found $r_{10} = 0.130$, $r_{20} = 0.732$ and $\rho = 0.862$ seem also in reasonable agreement with the known values [16].

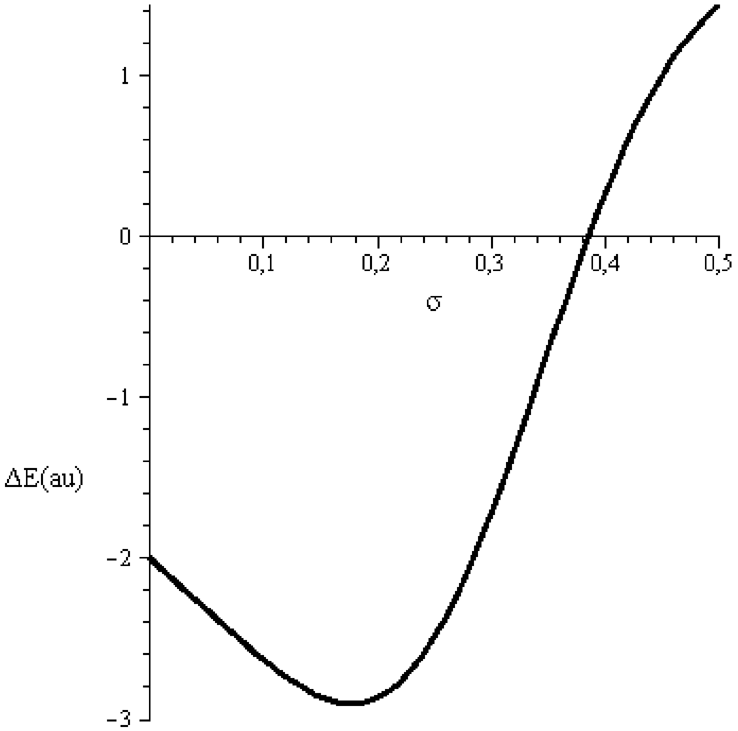

Fig1. Excess energy variation ΔE in au against the dimensionless parameter σ.

4. CONCLUSION

In this work we have considered a 2D formulation of the Helium Atom, derived a four-spinor Dirac-like equation and found the suitable matrices. The work is developed within two methods of approach: on the one hand through a total Hamiltonian in a Hylleraas context that ends in an extremum problem to be solved in a next paper. And on the other hand through a pair of Hamiltonians for an ion-atom and for an invader electron respectively. This second approach stands for a process controlled by a macro parameter of variation which is connected with the average values of the radial variables and that contains the ion helium atom ground state as a limit case. For this case we have discussed the general structure of the equations, separated the system of equations, found the angular eigenfunctions that decouple the system and a solution for the radial equation, in the approximation of constant inter-electron distance. This has made possible to calculate the ground state energy eigenvalue, whose value agrees with the experimental data within 0.1 % of accuracy.

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