

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

ABSTRACT

We present a two-dimensional analysis of the two-electron problem which comes from the classical conservation theorems and from which we obtain a version of the Dirac equation for the helium atom. Approximate solutions for this equation are discussed in two different methods, although in principle it can be solved analytically. One method is variational, of the Hylleraas type, the execution of which is left for a later communication. In contrast, the other method will have a more complete treatment, in which the set of equations will be separated into its angular and radial components. Furthermore, an exact solution for the angular component will be displayed as well as an approximate solution for the radial component, valid only for the fundamental state of the atom.

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

1. INTRODUCTION

Since the beginning of quantum chemistry in the 1920s the implementation of purely computational calculations of the Hartree-Fock type [1] has prevailed, due to their high performance and easy implementation, over more analytical structures such as those of the Hylleraas type [2]. Nevertheless some authors have tried to give an analytical basis to their iterative calculations, some of which have become the source of inspiration to start this line of work [3-6].

Following this analytical aim [7,8], we try to explore the Classical Theorems of Conservation *before* any quantization procedure is performed. We believe that they can reduce the dimensions of the coordinate systems that are necessary to formulate the problem in the quantum domain. More recently [9], we demonstrated that it is possible to use, in the analytical solution of the Dirac equation [10] for the hydrogen atom, Dirac 2x2 matrices rather than the usual 4x4 matrices, which leads to a considerable reduction in complexity of the problem. Moreover, our method led us to a new approach to the relativistic Hylleraas procedure in which the Dirac equation is derived from an extremum problem. This procedure was used to carry out numeric calculations for hydrogen-like atoms that resulted in extremely accurate energy eigenvalues with respect to the exact values, which are well known [11].

33 In this paper we treat the problem of the helium atom in a similar way to what we did in the case of the
 34 hydrogen atom. This treatment has allowed us to use Dirac 4x4 matrices instead of the 16x16 matrices of
 35 the Breit theory for the same atom [12], although it should be mentioned that we do not consider here the
 36 time retardation effects. Therefore we have developed a dual procedure: on the one hand we obtain a
 37 Dirac-like system of partial differential equations and on the other a Lagrangian density to carry out a
 38 variational calculation of the Hylleraas type, whose execution is however left to an upcoming article.

39
 40 For the Dirac-like procedure we take into account the trivial fact of the Theory of Relativity that we cannot
 41 add together the geodesics of individual particles. Then we consider a system formed by a single electron
 42 plus the nucleus, i.e., the He^+ ion, as a substrate on which an outer electron is introduced gradually
 43 through a penetration parameter. The gradual superposition of the corresponding Hamiltonians yields a
 44 system of differential equations that is dependent on the parameter of penetration, which should be used
 45 at the end of the calculation to obtain the minimum energy of the two-electron system. Considering now
 46 the Hylleraas-like procedure, the Hamiltonian is used in the traditional way in which the system is treated
 47 as a whole, without distinction of individual equations for each electron. For both procedures we try to
 48 express the system of equations in a truly covariant form, in which we can introduce later the retardation
 49 effects without breaking this fundamental requirement of the Theory of Relativity.

50
 51 In the last section of the paper we separate the angular and radial components of the Dirac-like system of
 52 partial differential equations for the helium atom [13]. We find the angular eigenfunctions that allow us to
 53 separate the system of radial equations and an asymptotic form of the wave function that is a solution of
 54 this system for the ground state of the atom. From this we get a determination of the atom energy
 55 eigenvalue that agrees with the experimental data within 0.1% of accuracy and we also check that it
 56 tends to the exact value of the ion energy when the outer electron is displaced to infinity.

57
 58
 59 **2. THEORY**

60
 61 In the infinity mass nucleus rest frame, the relativistic classical Hamiltonians for the individual electrons of
 62 the Helium atom in natural units $\hbar = c = 1$ and $\alpha = e^2 \cong 1/137$ are

63
$$H_1 = \sqrt{\mathbf{p}_1^2 + m^2} - \frac{2\alpha}{r_1} + \frac{\alpha}{r_{12}}, \quad H_2 = \sqrt{\mathbf{p}_2^2 + m^2} - \frac{2\alpha}{r_2} + \frac{\alpha}{r_{12}}, \quad (1a,b)$$

64 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
 65 case, on the other hand, if we consider the energy of the whole system, not taking into account the
 66 electrons individually, we arrive at the usual classical Hamiltonian

67
$$H = \sqrt{\mathbf{p}_1^2 + m^2} + \sqrt{\mathbf{p}_2^2 + m^2} - \frac{2\alpha}{r_1} - \frac{2\alpha}{r_2} + \frac{\alpha}{r_{12}}, \quad (1c)$$

68 in which the repulsion energy entries only once.

69

70 Still in the infinity mass nucleus rest frame, we choose to use a coordinate system in which the motion
71 occurs in the plane defined by the nucleus and the two electrons, i.e., $p_z = 0$, whose z axis may be
72 moving at constant velocity with respect to the z axis of another inertial system, so that the system is
73 invariant against space translations in this direction. In this frame, the only non vanishing components of
74 the classical angular momentum 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
75 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
76 $J_z = J_{1z} + J_{2z}$ respectively. Now, we know from Classical Mechanics [14] that the Poisson Bracket for
77 each electron angular momentum with respect to the Classical Hamiltonian (1c) is not null and that they
78 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
79 that the summation of them is null and hence the total angular momentum J_z becomes a constant of the
80 motion. This happens because the repulsion force between the electrons is a non central force and
81 hence it produces a torque in each electron that makes it oscillating about the axis that join the nucleus to
82 the other electron. In the Poisson Bracket it appears due to the implicit derivatives of $1/r_{12}$ with respect to
83 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
84 coordinates. Therefore, a 2D formulation of the problem is, at least in principle, perfectly possible and we
85 shall present two possibilities of it below.

86

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

$$91 \quad H_\sigma = (1 - \sigma)H_1 + 2\sigma H_2. \quad (1d)$$

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

99

100 We now search for a Dirac equation corresponding to the quantization of the classical Eqs. (1c) and (1d),
 101 in the infinity **mass** nucleus rest frame. The quantization is done in a way similar to that performed by
 102 Breit [12], in which each square root is "linearized" individually:

$$103 \quad \mathbf{p}_1^2 + m^2 = (\gamma^5 p_{1y} - \gamma^3 p_{1x} + m\gamma^0)^2, \quad (2a)$$

$$104 \quad \mathbf{p}_2^2 + m^2 = (\gamma^1 p_{2y} - \gamma^2 p_{2x} + m\gamma^0)^2. \quad (2b)$$

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

$$107 \quad \gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \boldsymbol{\gamma} = \begin{pmatrix} 0 & i\boldsymbol{\sigma} \\ -i\boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \gamma^5 = -i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (3)$$

108 where $\sigma_x, \sigma_y, \sigma_z$ are the Pauli spin matrices. As is well **known¹**, the γ matrices obey
 109 $\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\delta^{\mu\nu}$, for $\mu, \nu = 0, 1, 2, 3, 5$, that is, are unitary and anticommute in pairs, as required to
 110 make equal the two sides of Eqs.(2).
 111

112 By using the **momentum** operators $\mathbf{p}_1 = -i\nabla_1$ and $\mathbf{p}_2 = -i\nabla_2$, the linear Hamiltonian-like matrix
 113 operator associated with **Eq.(1c) and Eq.(1d)** becomes

$$114 \quad \hat{H} = i(\gamma^3\partial_{x_1} - \gamma^5\partial_{y_1}) - \frac{2\alpha}{r_1} + i(\gamma^2\partial_{x_2} - \gamma^1\partial_{y_2}) - \frac{2\alpha}{r_2} + 2m\gamma^0 + \frac{\alpha}{r_{12}}. \quad (4a)$$

$$115 \quad \hat{H}_\sigma = (1 - \sigma) \left[i(\gamma^3\partial_{x_1} - \gamma^5\partial_{y_1}) - \frac{2\alpha}{r_1} \right] + 2\sigma \left[i(\gamma^2\partial_{x_2} - \gamma^1\partial_{y_2}) - \frac{2\alpha}{r_2} \right] + (1 + \sigma) \left(m\gamma^0 + \frac{\alpha}{r_{12}} \right). \quad (4b)$$

116 In our coordinate system the total angular momentum **operator becomes the z component alone, i.e.**

$$117 \quad \hat{J}_z = iy_1\partial_{x_1} - ix_1\partial_{y_1} + iy_2\partial_{x_2} - ix_2\partial_{y_2}. \quad (5)$$

118 Now, as it is well known, the operator \hat{J}_z does not commute with \hat{H} or \hat{H}_σ . However, it can be verified
 119 immediately that total angular operator $\hat{M} = \hat{J}_z + \frac{1}{2}\alpha_{1z} + \frac{1}{2}\alpha_{2z}$, which includes the electron spins,
 120 commutes with both \hat{H} and \hat{H}_σ , that is $[\hat{H}, \hat{M}] = 0$ as well as $[\hat{H}_\sigma, \hat{M}] = 0$. Here, in the definition of

121 the operator \hat{M} were introduced the two-electron spin matrices $\alpha_{1,z} = -i\gamma^5\gamma^3 = \begin{pmatrix} -\sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}$ and

¹ There are several possibilities of defining these matrices according to the rules of the Clifford Algebra; we have chosen the only one that makes all products $\gamma^\mu\gamma^\nu$ to be real and positive along with γ^μ be diagonal for $\mu = 0$ and anti-diagonal for $\mu > 0$. These conditions are necessary for the Eq.(6b) and Eq.(8) below reduce to the one-electron 2D Dirac equation [9] when $\sigma \rightarrow 0$, which is a fundamental contour condition of our approach.

122 $\alpha_{2,z} = -i\gamma^2\gamma^1 = \begin{pmatrix} -\sigma_z & 0 \\ 0 & -\sigma_z \end{pmatrix}$ and the diagonalization problems to be solved become therefore $\hat{H}\psi = E\psi$

123 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.

124

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

127
$$\left[(\phi_{12} - E)\gamma^0 + i(\gamma^0\gamma^5\partial_{x_1} - \gamma^0\gamma^3\partial_{y_1}) + i(\gamma^0\gamma^1\partial_{x_2} - \gamma^0\gamma^2\partial_{y_2}) + 2m \right] \psi = 0, \quad (6a)$$

128
$$\left[(\phi_{12\sigma} - E)\gamma^0 + i(1-\sigma)(\gamma^0\gamma^5\partial_{x_1} - \gamma^0\gamma^3\partial_{y_1}) + 2i\sigma(\gamma^0\gamma^1\partial_{x_2} - \gamma^0\gamma^2\partial_{y_2}) + (1+\sigma)m \right] \psi = 0, \quad (6b)$$

129 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

130 functions. It may immediately be seen that Eqs.(6) can be put in the explicit covariant form

131
$$\left[\sigma_1\zeta_{1\mu}\pi_1^\mu + \sigma_2\zeta_{2\mu}\pi_2^\mu \right] \psi = 0$$
, by rewriting them in terms of the matrix operators $\zeta_{1\mu} = (1, -\gamma^0\gamma^5, \gamma^0\gamma^3, \gamma^0)$,

132 $\zeta_{2\mu} = (1, -\gamma^0\gamma^1, \gamma^0\gamma^2, \gamma^0)$ and the effective momentum operators

133
$$\hat{\pi}_k^\mu = \left(m, -i\partial_{x_k}, -i\partial_{y_k}, -\frac{2\alpha}{r_k} + \frac{\alpha}{\sigma_3 r_{12}} - \frac{E}{2\sigma_k} \right)$$
, where $k=1,2$; $\sigma_1 = \sigma_2 = 1$, $\sigma_3 = 2$ for (6a) and $\sigma_1 = 1 - \sigma$,

134 $\sigma_2 = 2\sigma$, $\sigma_3 = 1$ for (6b).

135

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

137
$$q_+\chi_1 - (\partial_{x_1} + i\partial_{y_1})\chi_3 + (-\partial_{x_2} + i\partial_{y_2})\chi_4 = 0, \quad (7a)$$

138
$$q_+\chi_2 + (\partial_{x_1} - i\partial_{y_1})\chi_4 - (\partial_{x_2} + i\partial_{y_2})\chi_3 = 0, \quad (7b)$$

139
$$q_-\chi_3 + (-\partial_{x_1} + i\partial_{y_1})\chi_1 + (-\partial_{x_2} + i\partial_{y_2})\chi_2 = 0, \quad (7c)$$

140
$$q_-\chi_4 + (\partial_{x_1} + i\partial_{y_1})\chi_2 - (\partial_{x_2} + i\partial_{y_2})\chi_1 = 0, \quad (7d)$$

141 and Eq.(6b) as well becomes

142
$$q_{\sigma+}\chi_1 - (1-\sigma)(\partial_{x_1} + i\partial_{y_1})\chi_3 + 2\sigma(-\partial_{x_2} + i\partial_{y_2})\chi_4 = 0, \quad (8a)$$

143
$$q_{\sigma+}\chi_2 + (1-\sigma)(\partial_{x_1} - i\partial_{y_1})\chi_4 - 2\sigma(\partial_{x_2} + i\partial_{y_2})\chi_3 = 0, \quad (8b)$$

144
$$q_{\sigma-}\chi_3 + (1-\sigma)(-\partial_{x_1} + i\partial_{y_1})\chi_1 + 2\sigma(-\partial_{x_2} + i\partial_{y_2})\chi_2 = 0, \quad (8c)$$

145
$$q_{\sigma-}\chi_4 + (1-\sigma)(\partial_{x_1} + i\partial_{y_1})\chi_2 - 2\sigma(\partial_{x_2} + i\partial_{y_2})\chi_1 = 0, \quad (8d)$$

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

148
 149 At this point we shall need to split the paper in two parts. In the first one, we shall present a variational
 150 version of Eqs.(7) that **allows** us to make numerical calculations of the energy eigenvalues in the
 151 Hylleraas scheme, as **we did** with high accuracy in the **case of one**-electron atoms [11]. But we shall only
 152 introduce the problem, which will be treated fully in a next paper. To do this, firstly we solve the last two
 153 equations of (7) for χ_3 and χ_4 , what yields

$$154 \quad \chi_3 = \frac{(\partial_{x_1} - i\partial_{y_1})\chi_1 + (\partial_{x_2} - i\partial_{y_2})\chi_2}{q_-}, \quad \chi_4 = \frac{-(\partial_{x_1} + i\partial_{y_1})\chi_2 + (\partial_{x_2} + i\partial_{y_2})\chi_1}{q_-}, \quad (9)$$

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

$$158 \quad L = \frac{|\partial_{x_1}\chi_1 - i\partial_{y_1}\chi_1|^2 + |\partial_{x_1}\chi_2 + i\partial_{y_1}\chi_2|^2 + |\partial_{x_2}\chi_1 + i\partial_{y_2}\chi_1|^2 + |\partial_{x_2}\chi_2 - i\partial_{y_2}\chi_2|^2}{q_-} + q_+ |\chi_1|^2 +$$

$$+ \Re \left[\frac{(\partial_{x_1}\chi_1^* + i\partial_{y_1}\chi_1^*)(\partial_{x_2}\chi_2 + i\partial_{y_2}\chi_2) - (\partial_{x_2}\chi_1^* + i\partial_{y_2}\chi_1^*)(\partial_{x_1}\chi_2 + i\partial_{y_1}\chi_2)}{q_-} \right] + q_+ |\chi_2|^2 \quad (10)$$

159 The extremum problem

$$160 \quad \delta \int L dx_1 dx_2 dy_1 dy_2 = 0 \quad (11)$$

161 is then solved, in the same way as done with the **hydrogen-like** atoms [11], by the requirement that the
 162 integral in (11) be stable against small variations of the algebraic forms of (χ_1, χ_2) about the
 163 corresponding exact solutions of (7) or some suitable approximation of them:

$$164 \quad \chi_\ell = \chi_{\ell ap} \sum_{\mu+\nu+\lambda=0}^N c_{\ell\mu\nu\lambda} r_1^\mu r_2^\nu r_{12}^\lambda \quad (12)$$

165 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
 166 coefficients corresponding to each function $\chi_{\ell ap}$ and N is the least integer necessary to a given order of
 167 precision to be reached. The variation becomes thus

$$168 \quad \left. \frac{\partial}{\partial c_{\ell\mu\nu\lambda}} \int L dx_1 dx_2 dy_1 dy_2 \right|_{N=0,1,2,\dots} = 0, \quad (13)$$

169 which produces two systems of linear equations in $c_{\ell\mu\nu\lambda}$, the determinants of which **generate** a
 170 polynomial function on the atom energy, the **roots of which** yield the energy eigenvalues for the atom. It

171 should be remarked that the need to know χ_{lap} in advance is in fact the great limitation of the Hylleraas
 172 methodology because, in practice, only asymptotic solutions are known, so that the use of arbitrary
 173 intermediary functions becomes the only way to perform the calculation. It is by this reason that we are
 174 proposing below the sigma variation procedure, in which we retain the almost exact form of the one-
 175 electron solution and perform the variation through a macro parameter that is related to the average
 176 values of the radial variables. The Hylleraas-like problem will be reconsidered formally in a next paper.

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 178
 179

3. APPROXIMATE GROUND STATE SOLUTION FOR THE SIGMA HAMILTONIAN

180 Now, considering the second part of the paper, we shall perform the variation through the parameter
 181 sigma which allows using **one-electron** solutions to provide an analytical approximation for the solution of
 182 the Eqs.(8). Thus, in order to separate the angular part of Eqs.(8), we must first address the angular
 183 momentum problem, $\hat{M}\psi = j\psi$, which written in the polar coordinates of the electrons 1 and 2
 184 becomes $(\partial_{\theta_1} + \partial_{\theta_2})\chi_k = i(j + \lambda_k)\chi_k$, where $\lambda_1 = 1$, $\lambda_2 = -1$, $\lambda_3 = \lambda_4 = 0$, are the diagonal values of
 185 $-\frac{1}{2}(\alpha_{1z} + \alpha_{2z})$ and $j = j_1 + j_2$. In accordance, the most general forms for the solutions of the angular
 186 equation are the set of eigenfunctions

$$187 \quad \chi_k = f_k e^{i\Phi_k}, \quad f_k = f_k(r_1, r_2, r_{12}), \quad k = 1, \dots, 4, \quad (14)$$

188 where the phase functions are

$$189 \quad \Phi_1 = (j_1 + \frac{1}{2})\theta_1 + (j_2 + \frac{1}{2})\theta_2 + g_1, \quad \Phi_2 = (j_1 - \frac{1}{2})\theta_1 + (j_2 - \frac{1}{2})\theta_2 + g_2, \quad (15a,b)$$

$$190 \quad \Phi_3 = (j_1 - \frac{1}{2})\theta_1 + (j_2 + \frac{1}{2})\theta_2 + g_3, \quad \Phi_4 = (j_1 + \frac{1}{2})\theta_1 + (j_2 - \frac{1}{2})\theta_2 + g_4, \quad (15c,d)$$

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

194

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

$$200 \quad \partial_{x_i} \pm i\partial_{y_i} = e^{\pm i\theta_i} \left(\partial_{r_i} \pm \frac{i}{r_i} \partial_{\theta_i} \right) + \frac{r_1 e^{\pm i\theta_1} - r_2 e^{\pm i\theta_2}}{r_{12}} \partial_{r_{12}}, \quad (16a)$$

201
$$\partial_{x_2} \pm i\partial_{y_2} = e^{\pm i\theta_2} \left(\partial_{r_2} \pm \frac{i}{r_2} \partial_{\theta_2} \right) - \frac{r_1 e^{\pm i\theta_1} - r_2 e^{\pm i\theta_2}}{r_{12}} \partial_{r_{12}}. \quad (16b)$$

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

206
 207 However, in this work, we shall limit ourselves to search for solutions satisfying the constraint $\rho = \langle r_{12} \rangle =$
 208 constant, so that in effect we arrive at $f_k = f_k(r_1, r_2)$ and further assume that $g_k = 0$, which will simplify
 209 considerably the resulting equations and also yields the variational relation $\rho = \rho(\sigma)$ that will be used to
 210 get the equilibrium configuration of the system. In these circumstances, we arrive at a unique system of
 211 equations given by the real part of (8), the imaginary one vanishing identically, that is

212
$$q_{\sigma+} f_1 - (1 - \sigma) \left(\frac{\partial f_3}{\partial r_1} + \frac{j_1 - \frac{1}{2}}{r_1} f_3 \right) - 2\sigma \left(\frac{\partial f_4}{\partial r_2} - \frac{j_2 - \frac{1}{2}}{r_2} f_4 \right) = 0, \quad (17a)$$

213
$$q_{\sigma+} f_2 + (1 - \sigma) \left(\frac{\partial f_4}{\partial r_1} + \frac{j_1 + \frac{1}{2}}{r_1} f_4 \right) - 2\sigma \left(\frac{\partial f_3}{\partial r_2} + \frac{j_2 + \frac{1}{2}}{r_2} f_3 \right) = 0, \quad (17b)$$

214
$$q_{\sigma-} f_3 - (1 - \sigma) \left(\frac{\partial f_1}{\partial r_1} + \frac{j_1 + \frac{1}{2}}{r_1} f_1 \right) - 2\sigma \left(\frac{\partial f_2}{\partial r_2} + \frac{j_2 - \frac{1}{2}}{r_2} f_2 \right) = 0, \quad (17c)$$

215
$$q_{\sigma-} f_4 + (1 - \sigma) \left(\frac{\partial f_2}{\partial r_1} - \frac{j_1 - \frac{1}{2}}{r_1} f_2 \right) - 2\sigma \left(\frac{\partial f_1}{\partial r_2} + \frac{j_2 + \frac{1}{2}}{r_2} f_1 \right) = 0. \quad (17d)$$

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

218
$$f_k = e^{-\beta_1 r_1 - \beta_2 r_2} \sum_{\mu+\nu=0}^1 a_{k\mu\nu} r_1^{s_1+\mu} r_2^{s_2+\nu}, \quad k = 1, 2, 3, 4, \quad (18)$$

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

222
$$\partial_{r_1} f_k = e^{-\beta_1 r_1 - \beta_2 r_2} \sum_{\mu+\nu=0}^1 a_{k\mu\nu} \left(\frac{s_1 + \mu}{r_1} - \beta_1 \right) r_1^{s_1+\mu-1} r_2^{s_2+\nu}, \quad k = 1, 2, 3, 4, \quad (19a)$$

223
$$\partial_{r_2} f_k = e^{-\beta_1 r_1 - \beta_2 r_2} \sum_{\mu+\nu=0}^1 a_{k\mu\nu} \left(\frac{s_2 + \nu}{r_2} - \beta_2 \right) r_1^{s_1+\mu} r_2^{s_2+\nu-1}, \quad (19b)$$

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

$$225 \quad \left[\gamma_{2\rho} - \frac{2\alpha(1-\sigma)}{r_1} - \frac{4\alpha\sigma}{r_2} \right] a_{1\mu\nu} + (1-\sigma) \left(\beta_1 + \frac{j_1 - s_1 - \frac{1}{2}}{r_1} \right) a_{3\mu\nu} + 2\sigma \left(\beta_2 + \frac{j_2 - s_2 - \frac{1}{2}}{r_2} \right) a_{4\mu\nu} = 0$$

$$226 \quad \tag{20a}$$

$$227 \quad \left[\gamma_{2\rho} - \frac{2\alpha(1-\sigma)}{r_1} - \frac{4\alpha\sigma}{r_2} \right] a_{2\mu\nu} + 2\sigma \left(\beta_2 - \frac{j_2 + s_2 + \frac{1}{2}}{r_2} \right) a_{3\mu\nu} + (1-\sigma) \left(\frac{j_1 + s_1 + \frac{1}{2}}{r_1} - \beta_1 \right) a_{4\mu\nu} = 0$$

$$228 \quad \tag{20b}$$

$$229 \quad \left[\gamma_{1\rho} + \frac{2\alpha(1-\sigma)}{r_1} + \frac{4\alpha\sigma}{r_2} \right] a_{3\mu\nu} + 2\sigma \left(\beta_2 + \frac{j_2 - s_2 - \frac{1}{2}}{r_2} \right) a_{2\mu\nu} + (1-\sigma) \left(\beta_1 - \frac{j_1 + s_1 + \frac{1}{2}}{r_1} \right) a_{1\mu\nu} = 0$$

$$230 \quad \tag{20c}$$

$$231 \quad \left[\gamma_{1\rho} + \frac{2\alpha(1-\sigma)}{r_1} + \frac{4\alpha\sigma}{r_2} \right] a_{4\mu\nu} - (1-\sigma) \left(\beta_1 + \frac{j_1 - s_1 - \frac{1}{2}}{r_1} \right) a_{2\mu\nu} + 2\sigma \left(\beta_2 - \frac{j_2 + s_2 + \frac{1}{2}}{r_2} \right) a_{1\mu\nu} = 0$$

$$232 \quad \tag{20d}$$

$$233 \quad \text{where } \gamma_{1\rho} = (1+\sigma)m + E - \frac{(1+\sigma)\alpha}{\rho} \text{ and } \gamma_{2\rho} = (1+\sigma)m - E + \frac{(1+\sigma)\alpha}{\rho}.$$

234

235 Now we start with the determination of the coefficients and parameters by observing that the system of
236 equations formed by each negative power $1/r_1$ and $1/r_2$ must vanish separately in order the coefficients

237 a_{k00} do not vanish:

$$238 \quad -2\alpha a_{100} + \left(j_1 - s_1 - \frac{1}{2} \right) a_{300} = 0, \tag{21a}$$

$$239 \quad -2\alpha a_{200} + \left(j_1 + s_1 + \frac{1}{2} \right) a_{400} = 0, \tag{21b}$$

$$240 \quad -\left(j_1 + s_1 + \frac{1}{2} \right) a_{100} + 2\alpha a_{300} = 0, \tag{21c}$$

$$241 \quad -\left(j_1 - s_1 - \frac{1}{2} \right) a_{200} + 2\alpha a_{400} = 0, \tag{21d}$$

242 and equally

$$243 \quad -4\alpha a_{100} + \left(j_2 - s_2 - \frac{1}{2} \right) a_{400} = 0, \tag{22a}$$

$$244 \quad -4\alpha a_{200} - \left(j_2 + s_2 + \frac{1}{2} \right) a_{300} = 0, \tag{22b}$$

$$245 \quad -\left(j_2 + s_2 + \frac{1}{2} \right) a_{100} + 4\alpha a_{400} = 0, \tag{22c}$$

$$246 \quad \left(j_2 - s_2 - \frac{1}{2} \right) a_{200} + 4\alpha a_{300} = 0. \tag{22d}$$

247 For this condition to be fulfilled it is necessary that the determinants of the systems (21) and (22) vanish,

248 from which we get $s_1 = -\frac{1}{2} + \sqrt{j_1^2 - 4\alpha^2}$ and $s_2 = -\frac{1}{2} + \sqrt{j_2^2 - 4\alpha^2}$.

249

250 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
 251 coefficients of the system of equations for the same powers, from which we get the system of recurrence
 252 equations

$$253 \quad \gamma_{2\rho}a_{100} + (1-\sigma)\beta_1a_{300} + 2\sigma\beta_2a_{400} - 2\alpha(1+\sigma)a_{110} - (1-\sigma)s_1a_{310} - 2\sigma s_2a_{410} = 0, \quad (23a)$$

$$254 \quad \gamma_{2\rho}a_{200} + 2\sigma\beta_2a_{300} + (1-\sigma)\beta_1a_{400} - 2\alpha(1+\sigma)a_{210} - 2\sigma s_2a_{310} + (1-\sigma)s_1a_{410} = 0, \quad (23b)$$

$$255 \quad (1-\sigma)\beta_1a_{100} + 2\sigma\beta_2a_{200} + \gamma_{1\rho}a_{300} + 2\alpha(1+\sigma)a_{310} - (1-\sigma)s_1a_{110} - 2\sigma s_2a_{210} = 0, \quad (23c)$$

$$256 \quad 2\sigma\beta_2a_{100} - (1-\sigma)\beta_1a_{200} + \gamma_{1\rho}a_{400} + 2\alpha(1+\sigma)a_{410} - 2\sigma s_2a_{110} + (1-\sigma)s_1a_{210} = 0. \quad (23d)$$

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

$$259 \quad \gamma_{2\rho}a_{100} + (1-\sigma)\beta_1a_{300} + 2\sigma\beta_2a_{400} = 0, \quad (25a)$$

$$260 \quad \gamma_{2\rho}a_{200} + 2\sigma\beta_2a_{300} + (1-\sigma)\beta_1a_{400} = 0, \quad (25b)$$

$$261 \quad (1-\sigma)\beta_1a_{100} + 2\sigma\beta_2a_{200} + \gamma_{1\rho}a_{300} = 0, \quad (25c)$$

$$262 \quad 2\sigma\beta_2a_{100} - (1-\sigma)\beta_1a_{200} + \gamma_{1\rho}a_{400} = 0, \quad (25d)$$

263 and also

$$264 \quad -2\alpha(1+\sigma)a_{110} - (1-\sigma)s_1a_{310} - 2\sigma s_2a_{410} = 0, \quad (26a)$$

$$265 \quad -2\alpha(1+\sigma)a_{210} - 2\sigma s_2a_{310} + (1-\sigma)s_1a_{410} = 0, \quad (26b)$$

$$266 \quad 2\alpha(1+\sigma)a_{310} - (1-\sigma)s_1a_{110} - 2\sigma s_2a_{210} = 0, \quad (26c)$$

$$267 \quad 2\alpha(1+\sigma)a_{410} - 2\sigma s_2a_{110} + (1-\sigma)s_1a_{210} = 0. \quad (26d)$$

268 Therefore in order the system (25) have a non trivial solution its determinant must vanish, from what we

269 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.

270

271 Now, the non trivial solution for the homogeneous system of equations (25) in the coefficients a_{k00} can be

272 obtained from the kernel associated to β_1 , whose basis is given by the two linearly independent column

273 vectors

$$274 \quad \psi_1 = \begin{pmatrix} -(1-\sigma)\beta_1 / \gamma_{2\rho} \\ -2\sigma\beta_2 / \gamma_{2\rho} \\ 1 \\ 0 \end{pmatrix}, \quad \psi_2 = \begin{pmatrix} -2\sigma\beta_2 / \gamma_{2\rho} \\ -(1-\sigma)\beta_1 / \gamma_{2\rho} \\ 0 \\ 1 \end{pmatrix}, \quad (27a,b)$$

275 out of which $\psi = a_{300}\psi_1 + a_{400}\psi_2$ is a general kernel vector. These basis vectors generate by its turn
 276 relations among the power series coefficients given by $a_{100} = -(1-\sigma)\beta_1 a_{300} / \gamma_{2\rho}$, $a_{200} = -2\sigma\beta_2 a_{300} / \gamma_{2\rho}$,
 277 $a_{400} = 0$ 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
 278 one.

279
 280 The last step in order to be able to make the evaluation of the energy eigenvalue of the system is as
 281 follows. First form a null line vector corresponding to the system (23), i.e., $R = [23a, 23b, 23c, 23d]$ and
 282 second make a contraction of it with one of the kernel vectors. Since it may be seen that both kernel
 283 vectors produce the same energy eigenvalue, so that the solutions in a_{300} and a_{400} are degenerated, we
 284 **have chosen** to make the contraction with the first kernel vector, that is, $R\psi_1 = 0$. This operation, as
 285 expected, eliminates the coefficients a_{k00} and produces a new relation connecting the coefficients a_{k10} :

$$286 \quad \left[\frac{2\alpha(1-\sigma^2)\beta_1}{\gamma_{2\rho}} - (1-\sigma)\left(\frac{3}{2} + s_1 + j_1\right) \right] a_{110} + 2\sigma \left[\frac{2\alpha(1+\sigma)\beta_2}{\gamma_{2\rho}} - \frac{3}{2} - s_2 + j_2 \right] a_{210} +$$

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

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

$$289 \quad - \left[\frac{2\alpha(1-\sigma^2)\beta_1}{\gamma_{2\rho}} - (1-\sigma)\left(\frac{1}{2} + s_1 + j_1\right) \right] \left((1-\sigma) \frac{\beta_1}{\gamma_{2\rho}} - 4\sigma^2 \left[\frac{2\alpha(1+\sigma)\beta_2}{\gamma_{2\rho}} - \frac{1}{2} - s_2 + j_2 \right] \frac{\beta_2}{\gamma_{2\rho}} + \right.$$

$$\left. + \left(\frac{1}{2} + s_1 - j_1\right) \frac{(1-\sigma)^2\beta_1}{\gamma_{2\rho}} + 4\sigma^2\beta_2 \left(\frac{1}{2} + s_2 + j_2\right) + 2\alpha(1+\sigma) \right) = 0. \quad (29)$$

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

$$293 \quad f_k = a_{k00} r_1^{s_1} r_2^{s_2} e^{-\beta_1 r_1 - \beta_2 r_2}, \quad k = 1, 2, 3, 4, \quad (30)$$

294 where we have redefined the coefficients a_{k00} as $a_{100} = -(1-\sigma)\beta_1 / \gamma_{2\rho}$, $a_{200} = -2\sigma\beta_2 / \gamma_{2\rho}$, $a_{300} = 1$ and
 295 $a_{400} = 0$.

296
 297 Now, we write by convenience $\beta_2 = h\beta_1$, where h is to be determined below. As a consequence,
 298 substituting β_1 found above and after a little of algebra, we get from (29)

299
$$\gamma_{1\rho}\gamma_{2\rho} = \frac{4\alpha^2(1+\sigma)^2[(1-\sigma)^2 + 4\sigma^2h^2](\gamma_{1\rho} - \gamma_{2\rho})^2}{(1-\sigma^2)(s_1 + \frac{1}{2}) + 4\sigma^2h(s_2 + \frac{3}{2})}, \quad (31)$$

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

303
$$E = \frac{\alpha(1+\sigma)}{\rho} + \frac{(1+\sigma)m}{\sqrt{1 + \frac{4\alpha^2(1+\sigma)^2[(1-\sigma)^2 + 4\sigma^2h^2]}{(1-\sigma^2)(s_1 + \frac{1}{2}) + 4\sigma^2h(s_2 + \frac{3}{2})}}}. \quad (32)$$

304 However, this is not yet the final step, since we still need to find out a value for h and the connection
 305 between σ and ρ , so that we can obtain a numerical evaluation of the atom energy. This is done by
 306 considering the values of the radii for which the probability given by the radial function (30) is a maximum,
 307 that is, for which the first derivatives (19) vanish. From this come the relations $r_{10} = s_1 / \beta_1$ and
 308 $r_{20} = s_2 / \beta_2$ among the most likely orbital radii and the points of maxima of the radial part of the wave
 309 function.

310
 311 Further we assume that $\rho = \langle r_{12} \rangle$ at the equilibrium configuration may be approximated by $\rho = r_{10} + r_{20}$
 312 and also a linear connection $r_{10} = \sigma r_{20}$ between the electron equilibrium radii which assures the contour
 313 condition $r_{20} \rightarrow \infty$ when $\sigma \rightarrow 0$. From these relations we finally get $h = \sigma s_2 / s_1$. At this point we have
 314 finally fulfilled all the steps toward getting an expression for the energy eigenvalues in terms of the basic
 315 electron properties along with the variation factor σ :

316
$$E = \frac{2\sigma m \alpha^2 (1+\sigma)^2}{C_1} + \frac{(1+\sigma)m}{C_2}, \quad (33)$$

317 where use has been made of the parameters

318
$$C_1 = \sqrt{[(1-\sigma)^2(s_1 + \frac{1}{2})s_1 + 4\sigma^3(s_2 + \frac{3}{2})s_2]^2 + 4\alpha^2(1+\sigma)^2[(1-\sigma)^2s_1^2 + 4\sigma^4s_2^2]}, \quad (34a)$$

319
$$C_2 = \sqrt{1 + \frac{4\alpha^2(1+\sigma)^2[(1-\sigma)^2s_1^2 + 4\sigma^4s_2^2]}{[(1-\sigma)^2(s_1 + \frac{1}{2})s_1 + 4\sigma^3(s_2 + \frac{3}{2})s_2]^2}}. \quad (34b)$$

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

322 equilibrium radii becomes $r_{10} = \frac{\sigma}{1+\sigma}\rho$ and $r_{20} = \frac{\rho}{1+\sigma}$.

323

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

$$328 \quad \Delta E = \frac{2\sigma(1+\sigma)^2}{C_1} + \left[\frac{(1+\sigma)}{C_2} - 1 - \sigma \right] \frac{1}{\alpha^2}, \quad (35)$$

$$329 \quad \rho = \frac{C_1}{2\sigma(1+\sigma)}. \quad (36)$$

330 The plot of the energy excess (in au) as a function of σ is shown in Fig.1, from which we immediately see
331 that the ion ground state limit $\Delta E = -2$ occurs for $\sigma = 0$ or $\rho = \infty$. The minimum of the energy excess for
332 $j_1 = j_2 = 1$ corresponds to the inner orbital state of the parahelium atom (or the state 1s-1s of the
333 Spectroscopy). By solving the equation $\frac{d}{d\sigma} \Delta E = 0$, we see that the equilibrium value occurs
334 approximately for $\sigma = 0.17753$, for whose value we get an energy ground state of $\Delta E = -2.9059$, which
335 agrees with the experimental value $\Delta E_{Exp} = -2.9033$ within 0.1% of accuracy. This means that the
336 approximations done to get the determination of the ground state energy of the atom, although rather
337 rough, were consistent with the dynamics of the physical system. Besides, the equilibrium radii found
338 $r_{10} = 0.130$, $r_{20} = 0.732$ and $\rho = 0.862$ seem also to be in a reasonable agreement with the known
339 values [15].

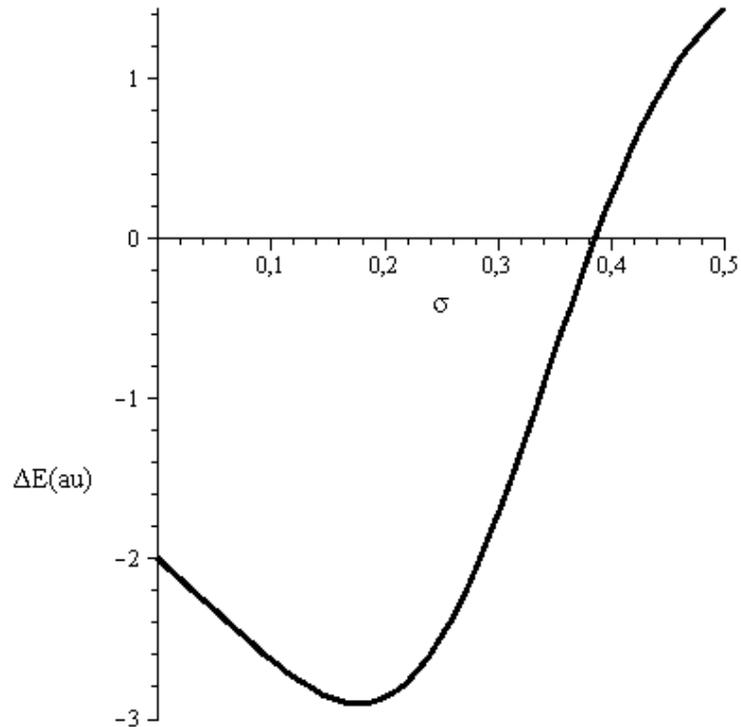


Fig1. Excess energy variation ΔE in au against the dimensionless parameter σ .

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4. CONCLUSION

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

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