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A Variational Approach for Numerically Solving the Two-Component Radial Dirac Equation for One-Particle Systems

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ABSTRACT

In this paper we propose a numerical approach to solve the relativistic Dirac equation suitable for computational calculations of one-electron systems. A variational procedure is carried out similar to the well-known Hylleraas computational method. An application of the method to hydrogen isoelectronic atoms is presented, showing its consistency and high accuracy, relative to the exact analytical eigenvalues.

1. Introduction

The study of hydrogen-like models plays an important role to test new approaches, and also in the description of the electronic structure of atomic and molecular systems. In this context, relativistic effects are of the most importance in a complete description of the physical system, mainly as the atomic mass of elements increases. Indeed, these effects play a crucial role in the description of the electronic structure of heavy elements.

Nevertheless, numerical methods used to take into account relativistic effects face several setbacks when the Dirac equation is used due to the existence of a negative continuum energy spectrum associated to the Dirac Hamiltonian operator, e.g., the appearance of instabilities in numerical calculations. Such methodologies are based on straight minimization of the expected values of the Dirac Hamiltonian with respect to a subset of the possible Dirac spinors [1-8]. As it is well known, it is very difficult to describe systems of many-electron atoms and molecules using the relativistic quantum mechanics approach. Even, in the Dirac's relativistic framework, where a one-electron spinorial solution is a two-vector whose components are scalar wave functions, the description is incomplete. Hence, a full relativistic description of the atomic and molecular electronic structure demands the application of Quantum Electrodynamics methods and consequently, the difficulty of implementing computational treatment for many-electron system increases. A survey of the currently available analytical solutions for relativistic one electron atoms may be found in Maple or Mathematica codes in [9,10] which may be valuable in comparing results of different theories.

In this paper, we propose an alternative approach that allows a simple numerical calculation to attain higher accuracy and allows comparison to other results. We improve the numerical methods to solve the Dirac equation, with special attention to the work of Drake and Goldman [11]. In this way we re-express the problem as one of finding the solution of the variation of a one-dimensional Lagrangean function. This Lagrangean is constructed as a positive definite function for particle energy eigenvalues, the antiparticle ones being get simply by sign reversion. This approach simplifies the procedure of finding the eigenvalues associated with a two-spinor subspace because it avoids automatically the variational collapse problem that always appears when considering the whole eigenvalue spectrum. The numerical procedure is done by calculating the algebraic variations of trial functions. This trial function we calculated in Section 3 for one-electron bound systems, *i.e.*, is similar to the Hylleraas computation method. Furthermore, the reduction to a two-dimensional Dirac-like equation is done by using transformation properties between noninertial frames, which will be useful in condensed matter such nanostructure, graphene and so on investigation. But for the applications in many-electrons as atomic and molecular systems the analytical equation given in [12] is not applicable. This paper goal is to obtain a numerical solution of the approach given in [12] to be useful in many-electrons applications. We should point out, as far we know

from the literature, our method to obtain the energy values of the Dirac-Coulomb problem derives directly from the Dirac equation and not from the usual minimization procedures of the Dirac Hamiltonian. In this context the results presented in the paper are new. Although the theoretical aspects have been discussed [12] in order to make the paper more self-contained, we devote Section 2 to a short review of the mathematical tools of that reference. In Section 3 we develop the numerical methods and apply them to hydrogen isoelectronic atoms showing its consistency and high accuracy, relative to the exact analytical eigenvalues. The conclusions are summarized in Section 4.

2. An Irreducible 2D Form for the Dirac Equation

The Dirac wave equation [13] is naturally associated with complex manifolds of the form $C^n \otimes C^n$, with $n \geq 1$. The usual 4D representation demands that $n = 2$ because the electron spin is introduced as an implicit or algebraic degree of freedom, which implies the need of four 4×4 linearly independent matrices to construct the standard 4-spinor Dirac equation. However, we will show here that an irreducible 2D representation is also possible in $C \otimes C$ for a hydrogen-like problem. In future we expect generalize the procedure for many electron problems, by considering other $C^n \otimes C^n$ sets.

Since objects of $C \otimes C$, that is the SU2 group are complex 2×2 quadratic matrices, [14] the corresponding wave function must be a two-spinor of the form $\psi = (\chi_1 \chi_2)$, so that we consider the stationary Hamiltonian problem

$$H(\chi_1, \chi_2) = E(\chi_1, \chi_2), \tag{2.1}$$

with

$$H = \varphi + i\sigma_y \partial_x - i\sigma_x \partial_y + \sigma_z m, \tag{2.2}$$

with $\sigma_i's$ being the usual Pauli matrices. In order to investigate what angular momentum corresponds to a constant of motion in this model we consider the z component of the angular moment vector

$$J_z = i(y\partial_x - x\partial_y). \tag{2.3}$$

Equation (2.3) can easily be verified that do not commute with the Hamiltonian H

$$[H, J_z] = \sigma_x \partial_x + \sigma_y \partial_y. \tag{2.4}$$

However, we should observe that

$$[H, J_z] = -2(\sigma_x \partial_x + \sigma_y \partial_y), \tag{2.5}$$

so that the effective operator,

$$M = J_z + \frac{1}{2}\sigma_z, \tag{2.6}$$

commutes with H and therefore is a constant of motion. In this context, M and H may be simultaneously diagonalized, that is

$$M(\chi_1, \chi_2) = j(\chi_1, \chi_2), \tag{2.7}$$

where j is an eigenvalue of M.

In order to check if our irreducible Dirac equation generates the correct one particle solution, we consider a Coulomb potential $\varphi(r) = -Z\alpha/r$, where Z is the nuclear charge and $\alpha \cong 1/137$ is the fine structure constant and determines the energy levels for hydrogenic atoms.

Equation (2.1) is explicitly written as a two component Dirac-like linear systems of equations

$$\partial_x \chi_1 + i\partial_y \chi_1 + q_- \chi_2 = 0 \tag{2.8a}$$

and

$$\partial_x \chi_2 - i\partial_y \chi_2 + q_- \chi_1 = 0, \tag{2.8b}$$

where we have introduced $q_\pm = m \pm (E + Z\alpha/r)$.

In ordinary polar coordinates (r, φ), the differential operators in Equations (2.7) and (2.8) become

$$\partial_x \pm i\partial_y = e^{\pm i\varphi}\left(\partial_r \pm ir^{-1}\partial_\varphi\right), \quad J_z = -i\partial_\varphi. \tag{2.9}$$

By substituting Equation (2.9) into Equation (2.7) and Equations (2.8), it is straightforward to verify that the general solutions are

$$\chi_1(r, \varphi) = e^{i\left(j-\frac{1}{2}\right)\varphi}R_1(r), R_1(r) = r^{-\frac{1}{2}}e^{-r}\sum_{\nu}^{n_0}a_{2\nu}r^{\nu+s} \tag{2.10a}$$

$$\chi_2(r, \varphi) = e^{i\left(j+\frac{1}{2}\right)\varphi}R_2(r), R_2(r) = r^{-\frac{1}{2}}e^{-r}\sum_{\nu}^{n_0}a_{2\nu+1}r^{\nu+s} \tag{2.10b}$$

The exact solution has recursion relations given by

$$a_{2\nu+2} = \frac{2(\nu - n + j)\left[\gamma_1(s + \nu + j + 1) + \gamma_2 Z\alpha\right]}{(\nu + 1)(2s + \nu + 1)\left[\gamma_1(s + \nu + j) + \gamma_2 Z\alpha\right]}a_{2\nu} \tag{2.11a}$$

$$a_{2\nu+1} = \frac{(j - \nu - s)\gamma_2 + \gamma_1 Z\alpha}{(s + \nu + j)\gamma_1 + \gamma_2 Z\alpha}a_{2\nu}, \tag{2.11b}$$

where $s = \sqrt{j^2 - Z^2\alpha^2}$, $a_0 = 1$, $0 \leq \nu \leq n_0 = n - j$ with $1 \leq j \leq n = 1, 2, \cdots$ The remaining parameters are given by $\gamma_1 = (m^2 - E^2)^{1/2}$ and $\gamma_2 = m - E$. Finally, Equations (2.11) form a polynomial solution of finite degree for Equations (2.7) and (2.8), if and only if, the corresponding energy eigenvalues are given exactly by

$$E_{n,j} = m\left[1 + \frac{Z^2\alpha^2}{\left(n - j + \sqrt{j^2 - Z^2\alpha^2}\right)^2}\right]^{-1/2} \tag{2.13}$$

$$\cong m\left\{1 - \frac{Z^2\alpha^2}{2n^2}\left[1 + \frac{Z^2\alpha^2}{n^2}\left(\frac{n}{j} - \frac{3}{4}\right)\right]\right\}$$

The first two radial functions $R_{1(n,j)}(r)$ and $R_{2(n,j)}(r)$ for the hydrogen ground state are

$$R_{1(1,1)} = r^{\frac{1}{2}}e^{-\gamma_1 r}, \qquad (2.14a)$$

$$R_{2(1,1)} = \frac{Z\alpha}{2}R_{1(1,1)}. \qquad (2.14b)$$

We would like to point out that the proportionality between $R_{2(n,j)}$ (the so called small component) and $R_{1(n,j)}$ (the so called large component) observed in Equation (2.14) occurs only when $n = j$; otherwise these functions are linearly independent.

3. Numerical Hylleraas-Like Variational Problem

We have seen in [12] that the method is analytically successful for one-electron atoms. We now formulate a numerical version, which is based in a Hylleraas-like variational approach given in [15], and aims to be extended to two or more electron systems in a future work. This time, instead of solving analytically the system composed of Equations (2.8), we isolate χ_2

$$\chi_2 = -\frac{\partial_x \chi_1 + i\partial_y \chi_1}{q_-}, \qquad (3.1)$$

and substitute into Equation (2.8b), obtaining

$$-\frac{(\partial_x - i\partial_y)(\partial_x \chi_1 + i\partial_y \chi_1)}{q_-} + q_+ \chi_1 = 0 \qquad (3.2)$$

We now express Equations (2.8) by means of an extremum problem in which the space integral of a general Lagrangean density $L(x, y, \chi(x,y), \partial^\mu \chi(x,y))$ is stationary against small algebraic variations in the form of $\chi(x, y)$ about the form of the exact eigenfunctions $\chi_1(x, y)$ and

$$\chi_1(r, \varphi) = e^{i(j-\frac{1}{2})\varphi} R_1(r), R_1(r) = r^{-\frac{1}{2}}e^{-r}\sum_\nu a_{2\nu} r^{\nu+s} \quad (3.3)$$

given by

$$\delta \int L \mathrm{d}x \mathrm{d}y = 0, \qquad (3.4)$$

which leads to the corresponding differential equation obeyed by the Lagrangean:

$$\partial_x \frac{\partial L}{\partial(\partial_x \chi^*)} + \partial_y \frac{\partial L}{\partial(\partial_y \chi^*)} - \frac{\partial L}{\partial \chi^*} = 0, \qquad (3.5)$$

where χ^* is the complex conjugate of χ that satisfies the asymptotic condition $\lim_{r\to\infty} \chi = 0$.

By comparing Equation (3.3) with Equation (3.5), it is clear that the only possible Lagrangean should be

$$L = \frac{(\partial_x \chi^* - i\partial_y \chi^*)(\partial_x \chi + i\partial_y \chi)}{q_-} + q_+ \chi^* \chi, \qquad (3.6)$$

For $\chi = \chi_1$, we recover Equation (2.10a) or, making use of Equation (2.9) one obtains Equations (2.8). Now we construct a variation function by a product of a power series and undetermined coefficients times the exact solution in Equation (2.10b)

$$\chi(r,\varphi) = e^{i(j-\frac{1}{2})\varphi} R_1'(r), R_1'(r) = R_1(r)\sum_{\nu=0}^{N} c_\nu r^\nu \qquad (3.7)$$

where N is an integer and to be specified later.

The variation process implied in Equation (3.4) is then performed directly, by requiring the vanishing of the partial derivatives of the integral of L with respect to the undetermined power series coefficients c_ν, whose values produce the algebraic variation of the form of $\chi(x, y)$ about the form of the exact eigenfunction $\chi_1(x, y)$, *i.e.*,

$$\delta \int L\mathrm{d}x\mathrm{d}y = 0 \implies \frac{\partial}{\partial c_\nu}\int_0^\infty\int_0^\infty L\mathrm{d}x\mathrm{d}y\bigg|_{\nu=0,1,2,\cdots} = 0. \quad (3.8)$$

More explicitly, after substituting Equation (3.7) into Equation (3.6), the modified Lagrangean becomes

$$L = \frac{1}{q_-}\left(\frac{\mathrm{d}R_1'}{\mathrm{d}r} - \frac{j-\frac{1}{2}}{r}R_1'\right)^2 + q_+ |R_1'|^2. \qquad (3.9)$$

Because the function $\chi_1(x, y)$ is not in general an eigenfunction of the Hamiltonian operator, Equation (3.7) does not lead naturally to a finite system of equations, as can be seen in Equation (2.8). Then it is necessary to truncate the power series of the modified function at same order of precision given by the integer N. In fact, Equation (3.7) leads us to an infinite system of linear equations such that the determinant must vanish in order to have a non trivial solution, so it has to be truncated, as usual in Hylleraas-like calculations, at a given order of precision [15]. The whole computational process is so simple that we could express and run the corresponding numerical algorithm using only what is available in Maple algebraic software.

The numerical results of energies $E'_{n,j} = E_{n,j} - m$ in atomic units are calculated for the ground state and several excited states of hydrogen atom and are given in **Table 1**, in which dED stands for the numerical deviation with respect to the exact analytical values given in Equation (2.13). To obtain these results we have used $N = 5$ in Equation (3.7) and 4 iterations. **Table 2** shows the set of

Table 1. Relativistic energy of the ground and excited states for several *n* and *j* quantum numbers of atomic hydrogen.

(n,j)	Energy (a.u.)	dED
1,1	−0.5000066564993	10^{-28}
2,1	−0.1250020801588	10^{-30}
2,2	−0.1250004160228	10^{-28}
3,1	−0.0555562951656	10^{-29}
3,2	−0.0555558020877	10^{-28}
3,3	−0.0555556377326	10^{-31}

Table 2. Set of fine structures with quantum number $n = 10$ for atomic hydrogen.

j	Energy (a.u.)	dED
1	–0.0050000246288	10^{-33}
2	–0.0050000113158	10^{-33}
3	–0.0050000068782	10^{-34}
4	–0.0050000046594	10^{-34}
5	–0.0050000033281	10^{-34}
6	–0.0050000024406	10^{-35}
7	–0.0050000018067	10^{-35}
8	–0.0050000013312	10^{-36}
9	–0.0050000009614	10^{-36}
10	–0.0050000006656	10^{-37}

fine structure levels for the quantum numbers $1 \le j \le n = 10$ of the hydrogen atom, where we have used $N = 7$ and the order of precision dED was obtained after 4 iterations.

The energy levels for several hydrogen isoelectronic atoms calculated by the present theory are shown in **Table 3**. In this table n_i is the number of iterations for a given order of precision, N is the truncation integer of the power series in Equation (3.7) and dED gives the comparative accuracy between the exact analytical Dirac solution and our numerical results. Using $N = 9$ to calculate the energy of Ba^{+55} we have obtained a precision of 10^{-14} against 10^{-31} for $N = 11$. In the case of U^{+91} we have obtained the precision of 10^{-9}, 10^{-23} and 10^{-31} for $N = 9$, $N = 11$ and $N = 15$, respectively. In order to improve precision, we only have to increase the value of N in the series in Equation (3.7). We can also observe in **Table 3** that when Z increases, the interaction is slower and it is necessary to increase N as well. In **Table 4** we compare the results obtained by our approach with the results found in the literature. The order of precision of our results (dED), in **Table 4**, is 10^{-30}. The numerical applications shown in **Tables 1-4** indicates that our method has a high numerical accuracy with respect to the analytical results obtained by Dirac.

4. Conclusions

In this paper, we have shown that there is an irreducible two dimensional representation for the Dirac equation whose analytical solution generates the same set of energy eigenvalues as the usual four dimensional representation and further that it makes possible to construct a numerical method which is a mirror of the Dirac differential equationn, from what comes highly accurate approximations for the energy eigenvalues. Finally we would like to stress that the novelty our method to obtain the energy values of the Dirac-Coulomb problem derives directly from the Dirac equation, and not from the usual minimization procedures of the Dirac Hamiltonian.

Table 3. Relativistic energy, in a.u. of the ground state of Hydrogen-like atoms ($Z = 1$ to $Z = 102$).

Z	E	Z	E
1	–0.50000665649931104731	52	–1404.52332758631590920033
2	–2.00010651249726432469	53	–1461.36026910371109997039
3	–4.50053929132519773443	54	–1519.47236640919919966336
4	–8.00170474475864392299	55	–1578.87254406089621996325
5	–12.50416297276934000740	56	–1639.57419426053935362067
6	–18.00863487201359360817	57	–1701.59119514188266563926
7	–24.51600271389592860677	58	–1764.93793011343325673707
8	–32.02731085329146217400	59	–1829.62930832754650488853
9	–40.54376656925865471232	60	–1895.68078635391592514576
10	–50.06674103932677960785	61	–1963.10839114209412224776
11	–60.59777044920055740614	62	–2031.92874436493159182838
12	–72.13855723998879545934	63	–2102.15908824279337936512
13	–84.69097149533550947742	64	–2173.81731295719291019458
14	–98.25705247111185728642	65	–2246.92198577216155288114
15	–112.83901027061631190355	66	–2321.49238199235796003527
16	–128.43922766852991613141	67	–2397.54851789873346275806
17	–145.06026208718432688168	68	–2475.11118581564566116752
18	–162.70484772902387112458	69	–2554.20199147780759832860
19	–181.37589786948026499118	70	–2634.84339388155204965554
20	–201.07650731483134086671	71	–2717.05874782278222061326
21	–221.80995502998452013686	72	–2800.87234934390344789463
22	–243.57970694151339488708	73	–2886.30948433425120450509
23	–266.38941892168328128383	74	–2973.39648055335419167421
24	–290.24293995963074038164	75	–3062.16076337414904511768
25	–315.14431552631471949691	76	–3152.63091557440060932916
26	–341.09779114033518422028	77	–3244.83674153954749771246
27	–368.10781614222108177221	78	–3338.80933627952974158030
28	–396.17904768532557004203	79	–3434.58115970649430380371
29	–425.31635495203522547714	80	–3532.18611667034913497971
30	–455.52482360460418166246	81	–3631.65964330580390542433
31	–486.80976040566885769484	82	–3733.03880030879780304143
32	–519.17669854336737806727	83	–3836.36237383324759053689
33	–552.63140209957351497559	84	–3941.67098478223553581684
34	–622.82835290147321496537	85	–4049.00720736272845231826
35	–622.82835290147321496537	86	–4158.41569788160634186484
36	–659.58333641184725776359	87	–4269.94333488547301321179
37	–697.45157045185898633610	88	–4383.63937189014906906161
38	–736.44006453090074108181	89	–4499.55560411116770335400
39	–776.55609714490997609037	90	–4617.74655079791051944820
40	–817.80722325073995296804	91	–4738.26965499593058096372
41	–860.20128213121596227370	92	–4861.18550282018289997370
42	–903.74640567162123886752	93	–4986.55806462318954241569
43	–948.45102706982318223631	94	–5114.45496079496754079159
44	–994.32389000383139426329	95	–5244.94775534605712340551
45	–1041.37405828228495485475	96	–5378.11228091373950661353
46	–1089.61092600520890335188	97	–5514.02899940997844856861
47	–1139.04422826437192218967	98	–5652.78340321689473490570
48	–1189.68405241473291995776	99	–5794.46646265550794426452
49	–1241.54084995079928423130	100	–5939.17512643585965958947
50	–1294.62544902425141021594	101	–6087.01288297896294345992
51	–1348.94906764193599311547	102	–6238.09039193074855081178

Table 4. Relativistic energy of the ground state of Hydrogen-like atoms (*Z* = 2, 10, 24, 26, 50, 90 and 110) results by this work and by others authors.

Ion	Energy (a.u.)		
	This work	Others authors	
He^+	−2.000106512497	−2.000106514	Ref. [7]
Ne^{+9}	−50.06674103932	−50.066742026	Ref. [8]
Cr^{23+}	−290.2429399596	−290.2428	Ref. [7]
Fe^{25+}	−341.0977911403	−341.097839	Ref. [4]
Sn^{+49}	−1294.625449024	−1294.62590	Ref. [8]
Th^{89+}	−4617.746550797	−4617.75	Ref. [7]
		−4616.45451	Ref. [8]
Ds^{109+}	−7579.653261351	−7579.69	Ref. [6]
		−7549.57702	Ref. [8]

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