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Variational representation of the Dirac-Coulomb Hamiltonian with no spurious roots

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A new approach to the variational representation of the Dirac equation is presented. The method takes advantage of the conditions satisfied by the eigenfunctions at the origin. In this way, a variational representation of the complete Dirac-Coulomb spectrum *without spurious roots* is obtained. Rigorous proofs of bounds for the positive and negative variational eigenvalues, as well as differential and integral properties of the variational eigenfunctions, are given. An alternative approach to the elimination of spurious roots based on constraining the basis set to satisfy the right nonrelativistic limit is also presented.

I. INTRODUCTION

In nonrelativistic quantum mechanics, variational methods provide a powerful technique for the construction of approximate eigenvalues and eigenfunctions and for calculations involving sums over the complete energy spectrum. The variational method cannot be trivially extended to the relativistic case because the Dirac Hamiltonian is not bounded from below. Any positive energy eigenvalue can collapse into a negative-energy eigenvalue as the basis set is increased or as the nonlinear parameters of the basis set are varied.

This paper is restricted to the case of an electron in a Coulomb potential $V(r)=-Ze^2/r$. In the present work we obtain a variational representation of the Dirac Hamiltonian without spurious roots, with a general proof of bounds for the energy eigenvalues.

To review briefly, the Dirac equation in the case of a Coulomb potential can be written as[1]

$$H\Psi=E\Psi \tag{1.1}$$

with

$$H=c\boldsymbol{\alpha}\cdot\mathbf{p}+\beta mc^2-\frac{Ze^2}{r}\ , \tag{1.2}$$

where $\boldsymbol{\alpha}$ and β are the usual 4×4 Dirac matrices. The solutions to (1.2) can be written in the form

$$\psi=\begin{bmatrix} i\dfrac{g(r)}{r}\Omega_{jlM} \\ -\dfrac{f(r)}{r}\Omega_{j\tilde{l}M}\end{bmatrix},\quad \tilde{l}=2j-1 \tag{1.3}$$

where $g(r)$ and $f(r)$ are the large and small radial functions and Ω_{jlM} is a two-component spherical spinor.

The large and small components satisfy the coupled equations

$$\begin{aligned}\left[\frac{1}{\alpha}-\frac{\alpha Z}{r}\right]g+\left[\frac{\kappa}{r}-\frac{d}{dr}\right]f&=\alpha Eg\ ,\\ \left[\frac{d}{dr}+\frac{\kappa}{r}\right]g-\left[\frac{1}{\alpha}+\frac{\alpha Z}{r}\right]f&=\alpha Ef\end{aligned} \tag{1.4}$$

in atomic units. κ is the Dirac quantum number $\kappa=\pm(j+\frac{1}{2})$ for $l=j\pm\frac{1}{2}$.

Defining a two-component radial spinor

$$\Phi=\begin{bmatrix} g(r) \\ f(r)\end{bmatrix}, \tag{1.5}$$

the system of equations (1.4) can be rewritten in Hamiltonian form as

$$H_r\Phi=E\Phi\ , \tag{1.6}$$

with the radial Hamiltonian H_r given by

$$\alpha H_r=\begin{bmatrix} \dfrac{1}{\alpha}-\dfrac{\alpha Z}{r} & \dfrac{\kappa}{r}-\dfrac{d}{dr} \\ \dfrac{d}{dr}+\dfrac{\kappa}{r} & -\dfrac{1}{\alpha}-\dfrac{\alpha Z}{r}\end{bmatrix}. \tag{1.7}$$

The exact positive energy solutions to (1.6) can be written in the form

$$\Phi_{n,\kappa}=r^{\gamma}e^{-\lambda_n r}\sum_{i=1}^{N}r^i\left[\begin{bmatrix} a_i \\ 0\end{bmatrix}+\begin{bmatrix} 0 \\ b_i\end{bmatrix}\right], \tag{1.8}$$

where a_i and b_i are constants, $N=n-1$ for $\kappa<0$ and $N=n$ for $\kappa>0$, and

$$\gamma=[\kappa^2-(\alpha Z)^2]^{1/2} . \tag{1.9}$$

In a previous work,[2] Drake and Goldman introduced a variational basis set of the form

$$g_i=r^{\gamma+i}e^{-\lambda r}\begin{bmatrix}1\\0\end{bmatrix},$$
$$f_i=r^{\gamma+i}e^{-\lambda r}\begin{bmatrix}0\\1\end{bmatrix},\quad i=0,1,2,\ldots,N-1 , \tag{1.10}$$

with λ an arbitrary positive nonlinear variational parameter. Their results can be summarized as follows.

(i) The $2N$ eigenvalues split into N-positive and N-negative eigenvalues.

(ii) The negative-energy eigenvalues all lie below $E=-\alpha^{-2}$ and move progressively up towards $-\alpha^{-2}$ as the basis dimension is increased.

(iii) The positive-energy eigenvalues behave exactly as if the Dirac Hamiltonian were a positive definite operator.

(iv) A spurious root appears in the case $\kappa>0$. This spurious root is degenerate with the lowest variational state of the same $|\kappa|$ but with $\kappa<0$.

The above properties of the set (1.10) were not proven rigorously by Drake and Goldman for a general basis set of dimension N, although an extensive numerical discussion of boundness and completeness was given.

In this work a new approach to the variational representation of the Dirac-Coulomb Hamiltonian is presented. The method takes advantage of the conditions satisfied by the eigenfunctions at the origin. In this way, a variational representation without spurious roots and a proof of a generalized Hylleraas-Undheim theorem[3] are obtained. As a consequence of this analysis a general proof of some of the properties of the basis set (1.10) is also obtained, including the presence and values of the spurious roots.

The zeroth-order conditions at the origin are first discussed in Sec. II. Section III presents a variational representation without spurious roots for which the right energy-bound properties and some general rules satisfied by the eigenfunctions are found. In Sec. IV an alternative approach to the elimination of spurious roots is introduced. This method is based on imposing the right nonrelativistic limit on the basis set.

II. THE ZEROTH-ORDER CONDITIONS AT THE ORIGIN

Consider an expansion of $g(r)$ and $f(r)$ in (1.4) around $r=0$. In general we can write

$$g(r)=r^{\mu}(g_0+g_1r+\cdots) ,$$
$$f(r)=r^{\mu}(f_0+f_1r+\cdots) . \tag{2.1}$$

To lowest order in r, as $r\to 0$, system (1.4) becomes

$$-\alpha Z g_0+(\kappa-\mu)f_0=0 ,$$
$$(\kappa+\mu)g_0-\alpha Z f_0=0 . \tag{2.2}$$

The solution to (2.2) yields

$$\mu=\gamma=[\kappa^2-(\alpha Z)^2]^{1/2} \tag{2.3}$$

and

$$\frac{g_0}{f_0}=\frac{\kappa-\gamma}{\alpha Z}=\frac{\alpha Z}{\kappa+\gamma}=q . \tag{2.4}$$

It is interesting to note that according to (2.4), the eigenfunctions of the Dirac Hamiltonian satisfy the *level-independent* constraint at the origin

$$\lim_{r\to 0}\frac{g(r)}{f(r)}=q=\frac{\kappa-\gamma}{\alpha Z} . \tag{2.5}$$

This ratio is the same for all eigenfunctions with the same value of κ.

Consider now the simplest basis set satisfying (2.5), i.e., the one-dimensional case

$$|\Psi_v\rangle=g(r)\begin{bmatrix}q\\1\end{bmatrix} . \tag{2.6}$$

Using (1.7) we obtain

$$\frac{\langle\Psi_v|H_r|\Psi_v\rangle}{\langle\Psi_v|\Psi_v\rangle}=\frac{1}{\alpha^2}\frac{q^2-1}{q^2+1}=-\frac{\gamma}{\alpha^2\kappa}\equiv\frac{\eta}{\alpha^2} . \tag{2.7}$$

A diagonalization of the Hamiltonian yields the same eigenvalue η regardless of the normalization function $g(r)$ used in (2.6). For $\kappa<0$, η is equal to the exact lowest positive eigenvalue α^2E_0 (e.g., $1s_{1/2}$, $2p_{3/2}$, etc.). For $\kappa>0$, η is a negative spurious root $\eta=-\alpha^2E_0$ lying in the forbidden energy gap.

Results (2.5) and (2.7) can also be obtained directly for the exact eigenstates. Defining $y(r)=g(r)/f(r)$, one obtains the following uncoupled differential equation for y:

$$\frac{dy}{dr}+\frac{2\kappa}{r}y-\left[\alpha E+\frac{\alpha Z}{r}+\frac{1}{\alpha}\right]-\left[\alpha E+\frac{\alpha Z}{r}-\frac{1}{\alpha}\right]y^2=0 .$$

For the exact eigenfunctions the result (2.7) is equivalent to the solution $y=\text{const}$, and the result (2.5) to $\lim_{r\to 0}y=\text{const}$.

Result (2.7) can be generalized to a basis set of arbitrary dimension. Consider the orthogonal set

$$|\Psi_n\rangle=(q^2+1)^{-1/2}\phi_n(r)\begin{bmatrix}q\\1\end{bmatrix},\quad n=1,2,\ldots,N$$
$$|\Psi_{N+m}\rangle=(q^2+1)^{-1/2}\theta_m(r)\begin{bmatrix}1\\-q\end{bmatrix},\quad m=1,2,\ldots,M \tag{2.8}$$

with

$$\langle\phi_i|\phi_j\rangle=\langle\theta_i|\theta_j\rangle=\delta_{ij} ,$$
$$\langle\phi_i|\phi_j\rangle=\int\phi_i\phi_j dr .$$

Using (1.7) we obtain

$$\langle \Psi_j \mid \alpha^2 H_r \mid \Psi_i \rangle = \eta \delta_{ij} ,$$

$$\langle \Psi_{N+n} \mid \alpha^2 H_r \mid \Psi_{N+m} \rangle = -\eta \delta_{nm} - 2\alpha^2 Z \left\langle \theta_n \left| \frac{1}{r} \right| \theta_m \right\rangle ,$$

$$\langle \Psi_j \mid \alpha^2 H_r \mid \Psi_{N+n} \rangle = \frac{\alpha Z}{\kappa} \langle \phi_j \mid \theta_n \rangle + \alpha\gamma \left\langle \phi_j \left| \frac{1}{r} \right| \theta_n \right\rangle + \alpha \left\langle \phi_j \left| \frac{d}{dr} \right| \theta_n \right\rangle ,$$

with $i,j = 1,2,\ldots,N$ and $n,m = 1,2,\ldots,M$.

The variational eigenvalues are obtained by solving $|\underline{H} - \lambda \underline{\mathbb{1}}| = 0$. Using an expansion in minors it is straightforward to show that for $N > M$ this determinant can be written as

$$|\underline{H} - \lambda \underline{\mathbb{1}}| = (\eta - \lambda)^{N-M} \left[\sum_{i=0}^{2M} b_i \lambda^i \right] .$$

In conclusion, there are at least $N - M$ degenerate eigenvalues $\lambda = \eta$; this result is independent of the functions used in the basis set (2.8). The variational eigenvalues do not cross as the nonlinear parameters of a basis set are continuously changed. It would appear then that for $N \geq M$, any positive eigenvalue λ greater than η cannot collapse below η as the nonlinear parameters of the basis set are changed. This result will be rigorously proved in the next section.

III. THE ZEROTH-ORDER VARIATIONAL BASIS SET

The results of the last section suggest that it may be advantageous to use the following decomposition of the radial Dirac eigenfunction:

$$|\Psi\rangle = (1+q^2)^{-1/2} \left[\phi \begin{bmatrix} q \\ 1 \end{bmatrix} + \theta \begin{bmatrix} 1 \\ -q \end{bmatrix} \right] , \tag{3.1}$$

instead of the usual one in large and small components. In the remainder of this paper ϕ and θ will be called the upper and lower components, respectively. ϕ and θ satisfy the following coupled equations:

$$\alpha \frac{d\theta}{dr} + \left[\frac{\alpha Z}{\kappa} + \frac{\alpha\gamma}{r} \right] \theta + (\eta - \epsilon)\phi = 0 , \tag{3.2a}$$

$$\alpha \frac{d\phi}{dr} - \left[\frac{\alpha Z}{\kappa} + \frac{\alpha\gamma}{r} \right] \phi + \left[\eta + \epsilon + \frac{2\alpha^2 Z}{r} \right] \theta = 0 , \tag{3.2b}$$

where $\epsilon = \alpha^2 E$.

Defining the new radial spinor as

$$\Phi(r) = \begin{bmatrix} \phi(r) \\ \theta(r) \end{bmatrix} , \tag{3.3}$$

the equations satisfied by ϕ and θ can be written in Hamiltonian form as

$$h\Phi = \epsilon\Phi \tag{3.4}$$

with

$$h = \begin{bmatrix} \eta & \frac{\alpha Z}{\kappa} + \frac{\alpha\gamma}{r} + \alpha\frac{d}{dr} \\ \frac{\alpha Z}{\kappa} + \frac{\alpha\gamma}{r} - \alpha\frac{d}{dr} & -\eta - \frac{2\alpha^2 Z}{r} \end{bmatrix} . \tag{3.5}$$

Notice that in (3.2) $\theta = 0$ is a valid solution for $\kappa < 0$ with eigenvalue $\epsilon = \eta$. In the case $\kappa > 0$ such a solution would yield a function ϕ diverging at infinity.

We introduce now a specific basis set that will force all the variational eigenfunctions to satisfy the zeroth-order condition (2.5) at the origin, and we will show that the variational eigenstates satisfy Eq. (3.2a) exactly. Consider the basis set

$$u_i = e^{-\lambda r} r^{\gamma+i} \begin{bmatrix} 1 \\ 0 \end{bmatrix} , \quad i = 0,1,2,\ldots,N \tag{3.6a}$$

$$w_j = e^{-\lambda r} r^{\gamma+j} \begin{bmatrix} 0 \\ 1 \end{bmatrix} , \quad j = 1,2,\ldots,N . \tag{3.6b}$$

Notice that any spinor Φ [Eq. (3.3)] constructed using the functions u_i and w_j in (3.6) will yield a Dirac wave function [Eq. (3.1)] that satisfies the condition (2.5) at the origin. This is achieved because the lowest power of r is γ for the u_i and $\gamma + 1$ for the w_j.

Using the functions u_i and w_j, we construct now the following basis set:

$$\sigma_i = \sum_{j=0}^{N} b_{ji} u_j = s_i(r) \begin{bmatrix} 1 \\ 0 \end{bmatrix} , \quad i = 0,1,2,\ldots,N \tag{3.7a}$$

$$\sigma_{i+N} = \sum_{j=1}^{N} c_{ji} w_j = t_i(r) \begin{bmatrix} 0 \\ 1 \end{bmatrix} , \quad i = 1,2,\ldots,N \tag{3.7b}$$

with

$$\langle s_i \mid s_j \rangle = \langle t_i \mid t_j \rangle = \delta_{ij} , \tag{3.8}$$

$$\langle s_i \mid s_j \rangle = \int s_i(r) s_j(r) dr . \tag{3.9}$$

Given the $2N+1$ orthonormal basis vectors σ_i, one obtains upon diagonalization of the Hamiltonian h, $2N+1$ variational eigenstates Φ_i which satisfy

$$\langle \Phi_i \mid h \mid \Phi_j \rangle = \epsilon_i \delta_{ij} , \quad i = 0,1,2,\ldots,2N \tag{3.10}$$

$$\langle \Phi_i \mid \Phi_j \rangle = \delta_{ij} , \tag{3.11}$$

with

$$|\Phi_i\rangle = \sum_{j=0}^{2N} |\sigma_j\rangle\langle\sigma_j \mid \Phi_i\rangle = \begin{bmatrix} \phi_i \\ \theta_i \end{bmatrix} . \tag{3.12}$$

We proceed now to investigate the properties of the variational radial functions ϕ_i and θ_i, and of the variational eigenvalues ϵ_i. Equation (3.10) can be rewritten as

$$|\Phi_i\rangle\langle\Phi_i \mid h - \epsilon_j \mid \Phi_j\rangle = 0 .$$

Summing over i, one obtains the following expression in terms of the orthonormal basis vectors σ_k:

$$\sum_{k=0}^{2N} |\sigma_k\rangle\langle\sigma_k|h-\epsilon_j|\Phi_j\rangle=0 .$$

Using (3.7), this expression is equivalent to the following two equations where we omit the index j:

$$\sum_{k=0}^{N} |s_k\rangle\langle s_k|A^+|\theta\rangle+(\eta-\epsilon)\sum_{k=0}^{N}|s_k\rangle\langle s_k|\phi\rangle=0 , \tag{3.13a}$$

$$\sum_{k=1}^{N} |t_k\rangle\langle t_k|A^-|\phi\rangle+\sum_{k=1}^{N}|t_k\rangle\langle t_k|v|\theta\rangle +(\eta+\epsilon)\sum_{k=1}^{N}|t_k\rangle\langle t_k|\theta\rangle=0 , \tag{3.13b}$$

with

$$A^{\pm}=\alpha\left[\frac{d}{dr}\pm\frac{Z}{\kappa}\pm\frac{\gamma}{r}\right] \tag{3.14}$$

and

$$v=\frac{\alpha^2 Z}{r} . \tag{3.15}$$

Due to the fact that the lowest power of r is $\gamma+1$ for the functions t_i and γ for the functions s_i, it follows that the lowest possible power of r in the radial variational functions θ and ϕ is $\gamma+1$ and γ, respectively. Then, by construction, we can write

$$A^+\theta=\sum_{i=0}^{M} p_i s_i , \tag{3.16}$$

where the p_i are constants, and then the set s_i completely represents $A^+\theta$, i.e.,

$$\sum_{k=0}^{N}|s_k\rangle\langle s_k|A^+|\theta\rangle=A^+|\theta\rangle . \tag{3.17}$$

The same is automatically true for the second term in (3.13a), i.e.,

$$\sum_{k=0}^{N}|s_k\rangle\langle s_k|\phi\rangle=|\phi\rangle .$$

We obtain then from (3.13a) the following important result:

$$\alpha\frac{d\theta}{dr}+\left[\frac{\alpha Z}{\kappa}+\frac{\alpha\gamma}{r}\right]\theta+(\eta-\epsilon)\phi=0 , \tag{3.18}$$

where ϕ and θ are the variational upper and lower radial functions, respectively. It is remarkable that both the variational and the exact eigenfunctions satisfy the same *differential* equation (3.18).

From (3.18) and (3.13) the following equations satisfied by θ and ϕ are obtained:

$$\alpha\left\langle\phi\left|\frac{d}{dr}\right|\theta\right\rangle+\frac{\alpha Z}{\kappa}\langle\phi|\theta\rangle+\frac{\gamma}{\alpha Z}\langle\phi|v|\theta\rangle+(\eta-\epsilon)\langle\phi|\phi\rangle=0 , \tag{3.19}$$

$$\alpha\left\langle\theta\left|\frac{d}{dr}\right|\phi\right\rangle-\frac{\alpha Z}{\kappa}\langle\theta|\phi\rangle-\frac{\gamma}{\alpha Z}\langle\theta|v|\phi\rangle+(\eta+\epsilon)\langle\theta|\theta\rangle+2\langle\theta|v|\theta\rangle=0 , \tag{3.20}$$

$$\frac{\alpha Z}{\kappa}\langle\theta|\theta\rangle+\frac{\gamma}{\alpha Z}\langle\theta|v|\theta\rangle+(\eta-\epsilon)\langle\theta|\phi\rangle=0 . \tag{3.21}$$

Having obtained the equations satisfied by the variational basis set, we proceed now to show that the variational energy spectrum has the proper bounds.

Using Eq. (3.11) in the form $\langle\phi|\phi\rangle+\langle\theta|\theta\rangle=1$, Eqs. (3.19) and (3.20) yield the following expression for the eigenvalues:

$$\epsilon=\frac{\eta+2\langle\theta|v|\theta\rangle}{1-2\langle\theta|\theta\rangle} , \tag{3.22}$$

which is valid for any variational eigenstate.

Calling $\epsilon_0=|\eta|$ we obtain for the case $\kappa<0$

$$\epsilon=\frac{\epsilon_0+2\langle\theta|v|\theta\rangle}{1-2\langle\theta|\theta\rangle} . \tag{3.23}$$

All the quantities involved in the right-hand side of Eq. (3.23) are positive, thus

$$\epsilon\geqq\epsilon_0 \text{ if } 0\leqq\langle\theta|\theta\rangle<\tfrac{1}{2} \tag{3.24}$$

and

$$\epsilon<-(\epsilon_0+2\langle\theta|v|\theta\rangle<-\epsilon_0 \text{ if } 1\geqq\langle\theta|\theta\rangle>\tfrac{1}{2} . \tag{3.25}$$

Equation (3.23) implies then that in the case $\kappa<0$, every positive variational eigenvalue is larger than or equal to the exact lowest possible energy $\epsilon_0=\gamma/|\kappa|$ for that value of κ. In other words, every positive variational eigenvalue is an upper bound to the ground state. In the Appendix we show that the negative eigenvalues are lower bounds to $-mc^2$ ($-1/\alpha^2$ in a.u.), i.e., $\epsilon^-<-1$.

We have then shown that in the case $\kappa<0$, no variational eigenvalue will lie in the forbidden gap. All the positive eigenvalues are upper bounds to ϵ_0, and all the negative eigenvalues are lower bounds to -1.

These results would not apply in principle to states with $\kappa>0$ because $\eta=-\epsilon_0$ in Eq. (3.22). However, we show now that if the same basis set is used for the cases $\kappa=\pm|\kappa|$, the resulting sets of eigenvalues are degenerate with the exception of the states with $\epsilon=\eta$.

Consider a specific variational eigenstate i with $\kappa<0$ and $\theta_i\neq0$, then according to (3.23):

$$\epsilon_i=\frac{\epsilon_0+2\langle\theta_i|v|\theta_i\rangle}{1-2\langle\theta_i|\theta_i\rangle} . \tag{2.6}$$

Defining now the function θ_i' as

$$\theta_i'=\pm\left[\frac{\langle\theta_i|v|\theta_i\rangle+\epsilon_0(1-\langle\theta_i|\theta_i\rangle)}{\langle\theta_i|v|\theta_i\rangle+\epsilon_0\langle\theta_i|\theta_i\rangle}\right]^{1/2}\theta_i \tag{3.27a}$$

or, correspondingly,

$$\theta_i=\pm\left[\frac{\langle\theta_i'|v|\theta_i'\rangle-\epsilon_0(1-\langle\theta_i'|\theta_i'\rangle)}{\langle\theta_i'|v|\theta_i'\rangle-\epsilon_0\langle\theta_i'|\theta_i'\rangle}\right]^{1/2}\theta_i' , \tag{3.27b}$$

and using (3.27) in Eq. (3.26) we obtain

$$\epsilon_i=\frac{-\epsilon_0+2\langle\theta_i'|v|\theta_i'\rangle}{1-2\langle\theta_i'|\theta_i'\rangle} . \tag{3.28}$$

But according to (3.22), Eq. (3.28) is the expression satisfied by a state with $\kappa>0$. θ_i' satisfies Eq. (3.28) with eigenvalue ϵ_i and ϕ_i' can be obtained from the differential equation (3.18) satisfied by the variational eigenstates. Equations (3.18) and (3.28) are simultaneously satisfied, implying that this is a variational solution of the eigenvalue equation (3.10). Since the variational solutions are unique, we conclude that for every state with quantum number κ, energy ϵ_i and lower component $\theta_i\neq 0$, there is a state with $\kappa'=-\kappa$, *the same energy,* and lower component

$$\theta_i'=\pm\left[\frac{\epsilon_i+\eta}{\epsilon_i-\eta}\right]^{1/2}\theta_i\ . \tag{3.29}$$

The last equation is obtained using Eq. (3.22). It is remarkable that the lower components of the degenerate levels with opposite signs of κ differ only by a constant. It follows from this degeneracy that all the results obtained for states with $\kappa<0$ and $\theta_i\neq 0$ apply identically to the states with $\kappa>0$. The states with $\theta=0$ are trivial in the sense that in this case the energy eigenvalue is a constant: $\epsilon=\epsilon_0$ for $\kappa<0$ and $\epsilon=-\epsilon_0$ for $\kappa>0$. This finishes the proof that the variational eigenvalues do not lie in the forbidden gap $\epsilon_0>\epsilon>-1$, with the exception of the spurious root $\epsilon=-\epsilon_0$ for the case $\kappa>0$.

We prove now that the number of positive- and negative-energy eigenvalues (excluding $\epsilon=\eta$) is the same.

Consider the $2N+1$-dimensional basis set introduced in (3.7) and call

$$\Phi_j^+=\begin{bmatrix}\phi_j^+\\ \theta_j^+\end{bmatrix},\quad j=1,2,\ldots,M$$

the set of eigenvalues with positive energies $\epsilon_j^+>\epsilon_0$. We show first that all the θ_j^+ are linearly independent. Suppose that θ_M^+ is linearly dependent on the other θ_j^+:

$$\theta_M^+=\sum_{j=1}^{M-1}c_j\theta_j^+\ .$$

We can define a vector

$$\mu=\Phi_M^+-\sum_{j=1}^{M-1}c_j\Phi_j^+$$

such that

$$\langle\mu\,|\,\mu\rangle=1+\sum_{j=1}^{M-1}c_j^2$$

where we used the fact that the ϕ_j^+ are orthonormal being eigenstates of the Hamiltonian, and

$$\frac{\langle\mu\,|\,h\,|\,\mu\rangle}{\langle\mu\,|\,\mu\rangle}=\left[\epsilon_M+\sum_{j=1}^{M-1}c_j^2\epsilon_j\right]\Big/\left[1+\sum_{j=1}^{M-1}c_j^2\right]>\epsilon_0\ . \tag{3.30}$$

Since μ is of the form

$$\mu=\begin{bmatrix}f\\ 0\end{bmatrix},$$

its eigenvalue should be ϵ_0. This contradicts Eq. (3.30) and we conclude that all the θ_j^+ are linearly independent. Similarly it can be proven that the lower component functions θ_j^- of the negative-energy states also are linearly independent. The only case in which both requirements are satisfied is when $N=M$. Then, excluding the state with $\epsilon=\eta$, there are as many positive as negative variational eigenvalues. In a similar way one can show that the ϕ_j^+ are linearly independent as well as the ϕ_j^-.

Still the problem of the spurious root $\epsilon=-\epsilon_0$ for states with $\kappa>0$ remains to be solved. We introduce now a modification to the basis set (3.7) that will eliminate the spurious root from the variational spectrum.

Equation (3.18) implies that for every variational eigenstate i with $\epsilon_i\neq\eta$,

$$\phi_i=\text{const}\times A^+\theta_i \tag{3.31}$$

with A^+ defined in (3.14). This proportionality suggests the introduction of the following basis set, which is a slight modification of the one presented in Eq. (3.6).

Define

$$w_i=e^{-\lambda r}r^{\gamma+i}\begin{bmatrix}0\\ 1\end{bmatrix},\quad i=1,2,\ldots,N \tag{3.32a}$$

$$v_j=A^+e^{-\lambda r}r^{\gamma+j}\begin{bmatrix}1\\ 0\end{bmatrix}$$

$$=\alpha\left[\frac{d}{dr}+\frac{Z}{\kappa}+\frac{\gamma}{r}\right]e^{-\lambda r}r^{\gamma+j}\begin{bmatrix}1\\ 0\end{bmatrix},\quad j=1,2,\ldots,N\ . \tag{3.32b}$$

For every state with $\epsilon_i\neq\eta$, the lower component θ_i will be a linear combination of the w_i and, by construction, the upper component ϕ_i will be the *same* linear combination of the v_j as stated by Eq. (3.31). [Notice that condition (3.17) is automatically satisfied by construction.] In other words, using the set (3.32) we obtain the same set of eigenvalues as with the previous basis set (3.6) with the exception that the eigenstate $\epsilon=\eta$ is now missing. All the proofs obtained until now for the basis set (3.6) apply identically to the basis set (3.32). The only difference between both sets is that the basis set (3.32) does not contain the spurious root $\epsilon=-\epsilon_0$ for the states with $\kappa>0$ as well as the ground state $\epsilon=\epsilon_0$ for the states with $\kappa<0$.

The ground state can be reintroduced in the case $\kappa<0$ by adding to the basis set (3.32) the vector

$$v_0=e^{-\lambda r}r^{\gamma}\begin{bmatrix}1\\ 0\end{bmatrix}\ . \tag{3.33}$$

The addition of this vector makes this set identical to the previous basis set (3.6) in the case $\kappa<0$. However, it is interesting to note that the exact (non-normalized) ground-state function

$$v_g=e^{-Zr/|\kappa|}r^{\gamma}\begin{bmatrix}1\\ 0\end{bmatrix} \tag{3.34}$$

can also be used, because v_g is orthogonal to all the other vectors in the set

$$\langle v_g \mid v_i \rangle = \alpha \int dr\, e^{-(\lambda + Z/|\kappa|)r} r^{2\gamma} \times [(2\gamma+i)r^{i-1} - (\lambda + Z/|\kappa|)r^i] = 0 \ . \tag{3.35}$$

Using Eq. (3.19) and

$$\Phi_g = \langle v_g \mid v_g \rangle^{-1/2} v_g \ , \tag{3.36}$$

Eq. (3.35) implies that

$$\langle \Phi_g \mid \Phi_i \rangle = 0$$

and

$$\langle \Phi_g \mid h \mid \Phi_i \rangle = 0 \ ,$$

so that Φ_g is a valid variational eigenstate with eigenvalue ϵ_0.

Finally it is shown now that the eigenvalue spectrum obtained using the basis set (3.32) satisfies a generalized Hylleraas-Undheim theorem.[3]

An infinite power expansion using the functions w_i of (3.32a) is a complete representation of the lower component of any exact eigenvector. In other words, as in the nonrelativistic case, for an exact eigenvector Φ_e there exists a set of linear coefficients c_i such that

$$\theta_e = e^{-\alpha r} r^\gamma \sum_{i=1}^{N} a_i r^i = e^{-\lambda r} r^\gamma \sum_{i=1}^{\infty} c_i r^i = \sum_{i=1}^{\infty} c_i w_i \ . \tag{3.37}$$

Such a linear combination will yield the exact eigenvalue ϵ_e as shown by Eq. (3.22). Using the fact that both the exact and the variational eigenfunctions satisfy the same differential equation (3.18), one obtains the following equivalent result for the upper component:

$$\phi_e = (\eta - \epsilon)^{-1} \sum_{i=1}^{\infty} c_i v_i \ , \tag{3.38}$$

where the c_i are the same as in (3.37). We conclude that the basis set (3.32), with (3.33) and (3.34) for the case $\kappa < 0$, is a complete representation of the exact wave functions when $N \to \infty$. In other words, as in the nonrelativistic case, the exact and variational spectra are the same when $N \to \infty$.

Consider now a variational basis set of dimension N. It is a general result of the diagonalization procedure that by adding a vector to the basis set, the resulting eigenvalues interleave with those of the smaller basis set.[4] In our case, adding a vector w_{N+1} (and then v_{N+1}) to the basis set (3.39) will yield a new set of eigenvalues, half positive and half negative. The interleaving of the positive- and of the negative-energy eigenvalues means that as the basis set dimension is increased, each positive eigenvalue decreases and each negative eigenvalue increases. We have shown that for an infinite dimension of the basis set the variational and exact bound-state spectra coincide, and that no eigenvalue lies in the forbidden gap. Then, as the dimension of the basis set is increased, each positive variational eigenvalue decreases towards the corresponding exact eigenvalue, and each negative eigenvalue increases towards $-mc^2$. In other words, we have a generalized Hylleraas-Undheim theorem: each positive eigenvalue is an upper bound to the exact eigenvalue and each negative eigenvalue is a lower bound to $-mc^2$.

We summarize now the results of this section. A basis set is introduced of the form

$$w_i = e^{-\lambda r} r^{\gamma+i} \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad i = 1,2,\ldots,N$$

$$v_i = [(2\gamma+i)/r + Z/\kappa - \lambda] e^{-\lambda r} r^{\gamma+i} \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad i = 1,2,\ldots,N$$

and in the case $\kappa < 0$, either v_0 or v_g are added to the set, with

$$v_g = e^{-Zr/|\kappa|} r^\gamma \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

and

$$v_0 = e^{-\lambda r} r^\gamma \begin{bmatrix} 1 \\ 0 \end{bmatrix} .$$

For this basis set, upon diagonalization of the Hamiltonian (3.5), the following results are found.

(i) The exact eigenvalue ϵ_0 is always present in the energy spectrum, in the case $\kappa < 0$.

(ii) The variational eigenvalues obtained in the cases $\kappa = |\kappa|$ and $\kappa = -|\kappa|$, excluding ϵ_0, are degenerate.

(iii) If a state with eigenvalue $\epsilon_i \neq \epsilon_0$ has lower component θ_i, then the corresponding state with the same energy and the opposite sign of κ will have a lower component

$$\theta_i' = \pm \left[\frac{\epsilon_i + \eta}{\epsilon_i - \eta} \right]^{1/2} \theta_i \ .$$

(iv) Every positive eigenvalue is an upper bound to the corresponding exact eigenvalue and every negative eigenvalue is a lower bound to $-mc^2$.

(v) The number of positive eigenvalues (excluding ϵ_0) and negative eigenvalues is the same.

(vi) There is no spurious root in the spectrum.

The following properties of the radial variational eigenfunctions can be obtained using the formulas of this section and the invariance of the norm of the Hamiltonian during diagonalization:

(a) $$\left\langle \theta_i \left| \frac{d}{dr} \right| \phi_i \right\rangle = \left\langle \theta_i' \left| \frac{d}{dr} \right| \phi_i' \right\rangle \ ,$$

(b) $$\hat{\sum} \langle \phi_i \mid \phi_i \rangle = \hat{\sum} \langle \theta_i \mid \theta_i \rangle = \hat{\sum} \langle \phi_i' \mid \phi_i' \rangle = \hat{\sum} \langle \theta_i' \mid \theta_i' \rangle = N \ ,$$

(c) $$\hat{\sum} \langle \theta_i \mid v \mid \theta_i \rangle = \hat{\sum} \langle \theta_i' \mid v \mid \theta_i' \rangle = -\tfrac{1}{2} \hat{\sum} \epsilon_i \ ,$$

(d) $$\hat{\sum} \left\langle \phi_i \left| \frac{d}{dr} \right| \theta_i \right\rangle = \hat{\sum} \left\langle \phi_i' \left| \frac{d}{dr} \right| \theta_i' \right\rangle = 0 \ ,$$

(e) $$\hat{\sum} \langle \phi_i \mid \theta_i \rangle = \hat{\sum} \langle \phi_i' \mid \theta_i' \rangle = 0 \ ,$$

(f) $$\hat{\sum} \langle \phi_i \mid v \mid \theta_i \rangle = \hat{\sum} \langle \phi_i' \mid v \mid \theta_i' \rangle = 0 \ ,$$

TABLE I. Variational eigenvalues for $s_{1/2}$ states for a hydrogenic ion with nuclear charge $Z=92$. The basis sets of Eqs. (1.10) and (3.7) were used for a and b, respectively. The exponential parameter was chosen to optimize the positive-energy level $n=4$.

n	a	b	Exact
6	1.007 947 103 2	1.006 015 528 5	0.993 232 093 9
5	0.990 422 849 9	0.990 396 323 5	0.990 122 665 8
4	0.984 277 125 6	0.984 277 125 6	0.984 277 125 6
3	0.971 297 594 2	0.971 296 235 5	0.971 292 560 3
2	0.933 303 950 4	0.933 187 369 2	0.933 041 992 6
1	0.746 291 088 3	0.741 134 719 8	0.741 134 719 8
1	−1.016 629 651 2	−1.017 195 862 2	
2	−1.029 469 965 2	−1.030 979 486 9	
3	−1.052 676 171 8	−1.056 987 963 8	
4	−1.103 074 067 0	−1.118 512 157 9	
5	−1.250 241 171 6	−1.342 560 994 4	
6	−2.101 462 320 2		

where $'$ denotes a change in the sign of κ, and

$$\hat{\Sigma} = \sum_{\epsilon_i \neq \epsilon_0} .$$

The sum rules are particularly useful to check numerically the computer program generating the basis set.

The completeness of the basis set has been checked numerically using relativistic electric-dipole sum rules.[5] In Table I we list the eigenvalues obtained for $s_{1/2}$ states for a hydrogenic ion with nuclear charge $Z=50$. A 12-dimensional basis set of the form (1.10) was used in the first column, and an 11-dimensional basis set of the form (3.32) and (3.33) was used in the second. The exponential parameter was chosen as to optimize the eigenvalue $n=4$. The same is done for $p_{1/2}$ states in the first two columns of Table II. Note the degeneracy of the eigenvalues with the corresponding ones in Table I.

With regard to the basis set (1.10), the methods of this section can be applied only in the case in which the number of powers used for the large and small components is the same. In this case Eq. (3.23) proves that (a) the basis set (1.10) yields positive eigenvalues that are upper bounds to the ground state, and (b) the states for opposite signs of κ are degenerate, including a spurious root for $\kappa>0$ degenerate with the lowest positive eigenvalue for $\kappa<0$. The discussion of Eq. (3.30) also applies in this case, showing that the set (1.10) will give the same number of positive and negative eigenvalues.

IV. THE FIRST-ORDER CONDITION AT THE ORIGIN

In this section an alternative method for the removal of spurious roots from the basis set (1.10) is presented. In a review paper, Kutzelnigg[6] relates spurious roots to wrong nonrelativistic limits. Following this idea, the spurious root of basis set (1.10) for the case $\kappa>0$ is removed by constraining the basis set to have the right nonrelativistic form in the limit $\alpha\rightarrow 0$.

Consider the ratio (2.4) at the origin. In the nonrelativistic limit for $\kappa>0$ we obtain

$$\lim_{\alpha\rightarrow 0}\frac{g_0}{f_0}=\frac{\alpha Z}{2\kappa} .$$

TABLE II. Variational eigenvalues for $p_{1/2}$ states for a hydrogenic ion with nuclear charge $Z=92$. The basis sets of Eqs. (1.10), (3.7), (4.3), and (4.3) and (4.4) were used for a, b, c, and d, respectively. The exponential parameter was chosen to optimize the positive-energy level $n=4$. The spurious root of set (1.10) is underlined.

n	a	b	c	d	Exact
6	1.007 947 103 2	1.006 015 528 5	1.005 225 185 4	1.005 633 224 2	0.993 232 093 9
5	0.990 422 849 9	0.990 396 323 5	0.990 384 289 0	0.990 390 640 8	0.990 122 665 8
4	0.984 277 125 6	0.984 277 125 6	0.984 277 125 6	0.984 277 125 6	0.984 277 125 6
3	0.971 297 594 2	0.971 296 235 5	0.971 295 719 8	0.971 295 987 3	0.971 292 560 3
2	0.933 303 950 4	0.933 187 369 2	0.933 152 405 6	0.933 170 294 7	0.933 041 992 6
1	<u>0.746 291 088 3</u>				
1	−1.016 629 651 2	−1.017 195 862 2	−1.016 705 144 7	−1.016 370 981 3	
2	−1.029 469 965 2	−1.030 979 486 9	−1.029 674 888 6	−1.028 801 673 1	
3	−1.052 676 171 8	−1.056 987 963 8	−1.053 280 250 2	−1.050 868 916 3	
4	−1.103 074 067 0	−1.118 512 157 9	−1.105 378 831 2	−1.097 292 622 1	
5	−1.250 241 171 6	−1.342 560 994 4	−1.266 326 957 3	−1.224 669 811 4	
6	−2.101 462 320 2			−1.919 623 088 2	

This equation reflects the fact that in the nonrelativistic limit, for $\kappa > 0$,

$$\lim_{r\to 0} g = r^{\kappa+1} .$$

In other words, the lowest-order coefficient for the expansion (2.1) of the large component in the nonrelativistic limit is g_1. The sufficient condition on g_1 can be obtained from the first-order conditions at the origin in system (1.4):

$$\begin{aligned} &g_0/\alpha - \alpha Z g_1 + (\kappa-\gamma-1) f_1 = \alpha E g_0 , \\ &(\kappa+\gamma+1) - g_1 f_0/\alpha + \alpha Z f_1 = \alpha E f_0 . \end{aligned} \tag{4.1}$$

From these equations we obtain the level-independent first-order condition for states with $\kappa > 0$:

$$(q+2\alpha Z) g_1 + (1-2\alpha Z q) f_1 = (2q/\alpha) f_0 . \tag{4.2}$$

From this equation, in the nonrelativistic limit we obtain

$$g_1 \sim f_1/\alpha ,$$

which is the sufficient condition to avoid the spurious root for $\kappa > 0$ in the basis set (1.10).

A basis set satisfying both the zeroth- and first-order conditions at the origin, can be constructed in the following way for states with $\kappa > 0$:

$$\begin{aligned} u_1 &= e^{-\lambda r} r^{\gamma} \begin{bmatrix} q + \dfrac{2(Z+\kappa\lambda)}{\alpha Z(1+2\kappa+2\gamma)} r \\ 1 \end{bmatrix} , \\ v_1 &= e^{-\lambda r} r^{\gamma} \begin{bmatrix} 1 \\ 1 + \dfrac{2q(Z+\kappa\lambda)}{\alpha Z(1-2\kappa+2\gamma)} r \end{bmatrix} , \\ u_i &= e^{-\lambda r} r^{\gamma+i} \begin{bmatrix} 1 \\ 0 \end{bmatrix} , \\ v_i &= e^{-\lambda r} r^{\gamma+i} \begin{bmatrix} 0 \\ 1 \end{bmatrix} , \quad i = 2,3,\ldots,N . \end{aligned} \tag{4.3}$$

This basis set provides a variational representation of the Dirac Hamiltonian (1.7) for the case $\kappa > 0$, without spurious roots. Although no formal proof of bounds for this basis set is provided, extensive numerical calculations have been done involving a wide range of dimensions of the basis set and values of the nonlinear parameter. In all cases one obtains that a diagonalization of (1.7) using the set (4.3) results in N-positive and N-negative eigenvalues which satisfy a generalized Hylleraas-Undheim theorem in the sense discussed in Sec. III. Completeness was checked numerically using the relativistic sum rules of Ref. 4.

The first-order condition at the origin (and then the right nonrelativistic limit) will still be satisfied if one does not force the zeroth-order condition at the origin to the states with $\kappa > 0$. This can be achieved by adding to the basis set (4.3) the vector

$$u_0 = e^{-\lambda r} r^{\gamma} \begin{bmatrix} 1 \\ 0 \end{bmatrix} . \tag{4.4}$$

The basis sets (4.3) and (4.4) will still satisfy the first-order condition (4.2). The same numerical results on bounds are obtained although now there is an extra negative-energy eigenstate which will accelerate the convergence of sum rules involving high powers of the energies. In the third and fourth columns of Table II, we list the results obtained for $p_{1/2}$ states using the basis sets (4.3) and (4.3) and (4.4), respectively.

V. DISCUSSION

We have shown that by introducing a separation of the wave function into "upper" and "lower" components, the Dirac equation with a Coulomb potential can be diagonalized in a suitably chosen finite basis set to obtain a discrete representation of the complete spectrum without spurious roots. This separation leads also to a rigorous proof of bounds for both the positive and negative variational eigenvalues. Also, by forcing the right nonrelativistic limit, we obtained a method for extracting, before diagonalization, the spurious roots from discrete basis sets that expand directly the "large" and "small" components of the wave function.

The basis set presented in Sec. III provides a very useful technique for calculations in which infinite summations over the complete relativistic spectrum are involved. A discussion of convergence for this type of calculations will be presented in a following paper.

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APPENDIX

In this appendix we prove that for the variational representation described in Sec. III, the negative eigenvalues are lower bounds to $-mc^2$. With the notation used in Sec. III, we show now that $|\epsilon^-| > 1$.

From Eq. (3.23) we obtain for the negative-energy eigenvalues:

$$|\epsilon^-| = \frac{\gamma/k + 2\langle\theta|v|\theta\rangle}{2\langle\gamma|\gamma\rangle - 1}, \quad k = |\kappa| , \tag{A1}$$

and using Eq. (3.21) we obtain

$$|\epsilon^-| = \frac{k/(2\alpha Z) + \alpha Z(2\langle\theta|\theta\rangle - 1)/(2k) - \gamma\langle\theta|\phi\rangle/k}{\gamma(2\langle\theta|\theta\rangle - 1)/(2\alpha Z) + \langle\theta|\phi\rangle} , \tag{A2}$$

where according to Eq. (3.25),

$$0 < 2\langle\theta|\theta\rangle - 1 \leq 1 . \tag{A3}$$

Consider in (A2) the case $\langle\theta|\phi\rangle = 0$:

$$|\epsilon^-|_{(\langle\theta|\phi\rangle=0)}=\frac{k}{\gamma(2\langle\theta|\theta\rangle-1)}+\frac{(\alpha Z)^2}{\kappa\gamma}>k/\gamma>1\ ,$$

together with the fact that in (A2), for any value of $\langle\theta|\theta\rangle$ $|\epsilon^-|$ is a monotonically decreasing function of $\langle\theta|\phi\rangle$, this implies that $|\epsilon^-|>1$ for any negative value of $\langle\theta|\phi\rangle$. We concentrate then from now on, on the case $\langle\theta|\phi\rangle>0$.

Using

$$\frac{\langle\theta|\phi\rangle}{(\langle\theta|\theta\rangle\langle\phi|\phi\rangle)^{1/2}}<1 \tag{A4}$$

and

$$\langle\theta|\theta\rangle+\langle\phi|\phi\rangle=1 \tag{A5}$$

together with Eq. (A2), we obtain the following lower bound for $|\epsilon^-|$:

$$|\epsilon^-|>x \tag{A6}$$

with

$$x=\frac{k/(2\alpha Z)+\alpha Z(2\langle\theta|\theta-1)/(2k)-(\gamma/k)[\langle\theta|\theta\rangle(1-\langle\theta|\theta\rangle)]^{1/2}}{\gamma(2\langle\theta|\theta\rangle-1)/2(\alpha Z)+[\langle\theta|\theta\rangle(1-\langle\theta|\theta\rangle)]^{1/2}}\ , \tag{A7}$$

where x is always positive because

$$k/(2\alpha Z)-(\gamma/k)[\langle\theta|\theta\rangle(1-\langle\theta|\theta\rangle)]^{1/2}$$
$$>k/(2\alpha Z)-\gamma/(2k)>0\ .$$

To simplify the notation in (A7) we define the new variable σ,

$$\sin\sigma=2\langle\theta|\theta\rangle-1,\quad 0<\sigma<\pi/2\ . \tag{A8}$$

With this substitution we can rewrite x in Eq. (A7) as

$$x(\sigma)=\frac{k/(\alpha Z)+(\alpha Z/k)\sin\sigma-(\gamma/k)\cos\sigma}{(\gamma/\alpha Z)\sin\sigma+\cos\sigma}\ ,$$
$$0<\sigma<\pi/2\ . \tag{A9}$$

Together with the condition $|\epsilon^-|>x$, we obtain from (A1)

$$|\epsilon^-|>y\ , \tag{A10}$$

where

$$y(\sigma)=\gamma/(k\sin\sigma),\quad 0<\sigma<\pi/2\ . \tag{A11}$$

Both conditions $|\epsilon^-|>x$ and $|\epsilon^-|>y$ are satisfied simultaneously; it follows then that

$$|\epsilon^-|>\max\{x,y\}\ . \tag{A12}$$

To analyze (A12) consider first the case $\sigma=\sigma_0$ for which $x(\sigma_0)=y(\sigma_0)$. From (A11) and (A9) we obtain

$$(\alpha Z/k)\sin\sigma_0-(\gamma/k)\cos\sigma_0=0\ , \tag{A13}$$

or

$$\sin\sigma_0=\gamma/k\ , \tag{A14}$$

and

$$x(\sigma_0)=y(\sigma_0)=1\ . \tag{A15}$$

But according to Eq. (A11), $y(\sigma)$ monotonically decreases with σ, then $|\epsilon^-|>1$ for $\sigma<\sigma_0$. We show now that in the region $\sigma>\sigma_0$, x is an increasing function of σ. Consider $x'=dx/d\sigma$,

$$x'=(\alpha Z)/k+\frac{(\alpha Z/k)\sin\sigma-(\gamma/k)\cos\sigma}{(\gamma/k)\sin\sigma+(\alpha Z/k)\cos\sigma}x\ , \tag{A16}$$

then, using (A13) we find $x'>(\alpha Z)/k>0$ for $\sigma>\sigma_0$. It follows then that $x(\sigma)>x(\sigma_0)$ for $\sigma>\sigma_0$, and then $|\epsilon^-|>1$ for $\sigma>\sigma_0$. Finally we obtain

$$\max\{x(\sigma),y(\sigma)\}>1,\quad 0<\sigma<\pi/2\ ,$$

and then

$$|\epsilon-|>1$$

as desired.

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