

Relativistic Sturmian basis functions

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The properties of relativistic one-electron Sturmian basis sets are discussed using Goscinski's definition of Sturmians rather than Rotenberg's. The potential-weighted orthonormality relations obeyed by the members of such a set are discussed. Weighted orthonormality relations in momentum space are also derived and used to construct a Sturmian expansion of the kernel of the momentum-space Dirac equation. The special case of spherical symmetry is discussed, and, as an illustrative example, relativistic Coulomb Sturmian basis sets are used to obtain solutions to the Dirac equation for an electron moving in a non-Coulomb potential.

1. Introduction

A Sturmian basis set is sometimes defined [13] as a set of solutions of the wave equation for some easily solved potential, $v_0(\mathbf{x})$, where, for each solution in the set, the potential has been weighted by a factor b_ν , especially chosen so that all the functions in the set will correspond to the same energy. Such a basis set can be shown to obey a potential-weighted orthonormality relation. Shull and Löwdin [20] originally introduced single-electron hydrogenlike Sturmian basis functions into quantum chemistry because these functions are complete without the inclusion of the continuum. The name "Sturmian" was introduced by Rotenberg [18] in order to emphasize the connection with Sturm–Liouville theory. Weniger [21] has studied the orthonormality and completeness properties of Sturmian basis sets and shown that such a set forms the basis of a Sobolev space. Herschbach and Avery [5,10] generalized the idea of Sturmian basis sets by introducing many-electron Sturmians. Recently, Aquilanti and Avery [2,8] developed methods for constructing many-electron Sturmians based on the actual external potential experienced by a collection of electrons in an atom or molecule, i.e., the attractive potential due to the nuclei. In the present paper, we will consider the properties of sets of solutions of the Dirac equation, where the potential has been weighted by a factor, b_ν , especially chosen so that all the functions in the set will correspond to the same energy. There exists a considerable literature [11,16] on relativistic Sturmian basis sets, but we hope that the present paper will nevertheless help to broaden our understanding of their properties.

2. Orthonormality relations

Let $\chi_\nu(\mathbf{x})$ represent a set of functions satisfying the one-electron Dirac equation for some electrostatic potential $v_0(\mathbf{x})$:

$$\left[i\hbar c \boldsymbol{\alpha} \cdot \frac{\partial}{\partial \mathbf{x}} - \gamma_0 m_0 c^2 + \varepsilon \right] \chi_\nu(\mathbf{x}) = b_\nu v_0(\mathbf{x}) \chi_\nu(\mathbf{x}). \quad (1)$$

The constant b_ν is a weighting factor especially chosen so that all the functions in the set will correspond to the same value of the one-electron energy, ε . The symbol $\boldsymbol{\alpha}$ represents the Dirac operator proportional to velocity, while γ_0 is defined by

$$\gamma_0 \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (2)$$

(Notice that the relativistic energy, ε , includes the rest energy, and that the terms in the Dirac equation have been rearranged.) The set of 4-component spinors defined in this way constitute a relativistic one-particle Sturmian basis set. Such a basis set obeys weighted orthonormality relations both in position-space and in momentum space. To see this, we can write the adjoint of equation (1) for some other member of the set, $\chi_{\nu'}$:

$$\chi_{\nu'}^\dagger(\mathbf{x}) \left[-i\hbar c \boldsymbol{\alpha} \cdot \frac{\partial}{\partial \mathbf{x}} - \gamma_0 m_0 c^2 + \varepsilon \right] = b_{\nu'} v_0(\mathbf{x}) \chi_{\nu'}^\dagger(\mathbf{x}). \quad (3)$$

If we multiply both sides of (3) from the right by χ_ν and both sides of (1) from the left by $\chi_{\nu'}^\dagger$, evaluate the scalar products, and subtract the two equations, making use of the Hermiticity of the operator in square brackets, we obtain

$$0 = (b_{\nu'} - b_\nu) \int d\mathbf{x} \chi_{\nu'}^\dagger(\mathbf{x}) v_0(\mathbf{x}) \chi_\nu(\mathbf{x}), \quad (4)$$

thus when $b_{\nu'} \neq b_\nu$ we must have the potential-weighted orthonormality relation

$$\int d\mathbf{x} \chi_{\nu'}^\dagger(\mathbf{x}) v_0(\mathbf{x}) \chi_\nu(\mathbf{x}) = 0. \quad (5)$$

This still does not tell us how to normalize the functions in the relativistic Sturmian basis set, but it will be convenient to normalize them in such a way that the set obeys the orthonormality relation

$$\int d\mathbf{x} \chi_{\nu'}^\dagger(\mathbf{x}) v_0(\mathbf{x}) \chi_\nu(\mathbf{x}) = -\frac{\varepsilon}{b_\nu} \delta_{\nu',\nu}. \quad (6)$$

An additional remark must be made in order to clarify the meaning of the orthonormality relations shown in equation (6): Since ν stands for a set of quantum numbers, there may be minor quantum numbers on which the value of b_ν does not depend. For

example, for systems with spherical symmetry, the quantum numbers corresponding to total angular momentum and its z -component are minor quantum numbers. Orthogonality of the basis functions corresponding to different values of the minor quantum numbers does not follow from equation (4), but must be established in some other way. The momentum-space orthonormality relations can be derived from (6) in the following way: We introduce the set of Fourier-transformed spinors defined by

$$\begin{aligned}\chi_\nu^t(\mathbf{p}) &\equiv \frac{1}{(2\pi)^{3/2}} \int d\mathbf{x} \chi_\nu(\mathbf{x}) e^{-i\mathbf{p}\cdot\mathbf{x}}, \\ \chi_\nu(\mathbf{x}) &\equiv \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p} \chi_\nu^t(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}}.\end{aligned}\quad (7)$$

If we introduce the Fourier transform expression into equation (1), we obtain

$$\frac{1}{(2\pi)^{3/2}} \int d\mathbf{p} [-\hbar c \boldsymbol{\alpha} \cdot \mathbf{p} - \gamma_0 m_0 c^2 + \varepsilon] \chi_\nu^t(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} = b_\nu v_0(\mathbf{x}) \chi_\nu(\mathbf{x}). \quad (8)$$

We next multiply both sides of (8) by $e^{-i\mathbf{p}'\cdot\mathbf{x}}/(2\pi)^{3/2}$ and integrate over $d\mathbf{x}$, which gives us

$$[-\hbar c \boldsymbol{\alpha} \cdot \mathbf{p}' - \gamma_0 m_0 c^2 + \varepsilon] \chi_\nu^t(\mathbf{p}') = \frac{b_\nu}{(2\pi)^{3/2}} \int d\mathbf{x} e^{-i\mathbf{p}'\cdot\mathbf{x}} v_0(\mathbf{x}) \chi_\nu(\mathbf{x}). \quad (9)$$

Then, using equations (6) and (9) and the fact that the position-space scalar product of two functions is equal to the momentum-space scalar product of their Fourier transforms, we have

$$\int d\mathbf{p} \chi_{\nu'}^{\dagger t}(\mathbf{p}) [-\hbar c \boldsymbol{\alpha} \cdot \mathbf{p} - \gamma_0 m_0 c^2 + \varepsilon] \chi_\nu^t(\mathbf{p}) = -\varepsilon \delta_{\nu',\nu}. \quad (10)$$

3. Sturmian expansion of the momentum-space Dirac equation's kernel

According to the Fourier convolution theorem, the Fourier transform of the product of two functions is the momentum-space convolution of their Fourier transforms. Applying this theorem to the right-hand side of equation (9), we obtain

$$[-\hbar c \boldsymbol{\alpha} \cdot \mathbf{p} - \gamma_0 m_0 c^2 + \varepsilon] \chi_\nu^t(\mathbf{p}) = \frac{b_\nu}{(2\pi)^{3/2}} \int d\mathbf{p}' v_0^t(\mathbf{p} - \mathbf{p}') \chi_\nu^t(\mathbf{p}'), \quad (11)$$

which is the momentum-space integral equation satisfied by the functions in our basis set. We now let

$$[-\hbar c \boldsymbol{\alpha} \cdot \mathbf{p} - \gamma_0 m_0 c^2 + \varepsilon] \chi_\nu^t(\mathbf{p}) \equiv \tilde{\chi}_\nu^t(\mathbf{p}). \quad (12)$$

Then (10) can be rewritten in form

$$\int d\mathbf{p} \chi_{\nu'}^{\dagger t}(\mathbf{p}) \tilde{\chi}_\nu^t(\mathbf{p}) = -\varepsilon \delta_{\nu',\nu} \quad (13)$$

while (11) becomes

$$\tilde{\chi}_\nu^t(\mathbf{p}) = \frac{b_\nu}{(2\pi)^{3/2}} \int d\mathbf{p}' v_0^t(\mathbf{p} - \mathbf{p}') \chi_\nu^t(\mathbf{p}'). \quad (14)$$

Equations (13) and (14) imply that the kernel of the integral equation can be expanded in the form

$$v_0^t(\mathbf{p} - \mathbf{p}') = - \sum_{\nu'} \frac{(2\pi)^{3/2}}{\varepsilon b_{\nu'}} \tilde{\chi}_{\nu'}^t(\mathbf{p}) \tilde{\chi}_{\nu'}^{\dagger t}(\mathbf{p}') \quad (15)$$

because, if we substitute (15) into the right-hand side of (14) and make use of the orthonormality relation (13), we obtain the left-hand side of (14).

4. Spherically symmetric potentials

If the potential is spherically symmetric, so that $v_0\mathbf{x} = v_0(r)$ then the Sturmian basis functions, $\chi_\nu(\mathbf{x})$, will have the form [1]

$$\chi_\nu(\mathbf{x}) = \begin{pmatrix} ig(r)\Omega_{jlm} \\ -f(r)\Omega_{j'l'm} \end{pmatrix}, \quad (16)$$

where

$$l' = 2j - l. \quad (17)$$

For $j = l + \frac{1}{2}$, the spherical spinors, Ω_{jlm} , are given by

$$\Omega_{jlm} = \begin{pmatrix} \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}} Y_{l,m-\frac{1}{2}}(\theta, \phi) \\ \sqrt{\frac{l-m+\frac{1}{2}}{2l+1}} Y_{l,m+\frac{1}{2}}(\theta, \phi) \end{pmatrix} \quad (18)$$

while for $j = l - \frac{1}{2}$,

$$\Omega_{jlm} = \begin{pmatrix} -\sqrt{\frac{l-m+\frac{1}{2}}{2l+1}} Y_{l,m-\frac{1}{2}}(\theta, \phi) \\ \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}} Y_{l,m+\frac{1}{2}}(\theta, \phi) \end{pmatrix}. \quad (19)$$

The radial functions $g(r)$ and $f(r)$ are solutions of the coupled differential equations

$$\begin{aligned} \frac{dg}{dr} + (1 + \kappa) \frac{g}{r} - \frac{1}{\hbar c} (\varepsilon + m_0 c^2 - v_0(r)) f &= 0, \\ \frac{df}{dr} + (1 - \kappa) \frac{f}{r} + \frac{1}{\hbar c} (\varepsilon - m_0 c^2 - v_0(r)) g &= 0, \end{aligned} \quad (20)$$

where

$$\kappa = \begin{cases} -(l + 1), & j = l + \frac{1}{2}, \\ l, & j = l - \frac{1}{2}. \end{cases} \quad (21)$$

The relativistic energy eigenvalues are determined by these coupled differential equations, together with the requirement that the wave function be normalizable.

5. Relativistic Coulomb Sturmians

In the special case where $v_0(r) = -e^2/r$ and

$$b_\nu v_0(r) = -\frac{b_\nu e^2}{r}, \quad (22)$$

the radial functions are given by [1]

$$\begin{aligned} g &= -\mathcal{N}r^{\gamma-1}e^{-b_\nu r/(Na_0)} \\ &\times \left\{ n_r F\left(-n_r + 1 \mid 2\gamma + 1 \mid \frac{2b_\nu r}{Na_0}\right) - (N - \kappa)F\left(-n_r \mid 2\gamma + 1 \mid \frac{2b_\nu r}{Na_0}\right) \right\}, \\ f &= -\mathcal{N}\mathcal{R}r^{\gamma-1}e^{-b_\nu r/(Na_0)} \\ &\times \left\{ n_r F\left(-n_r + 1 \mid 2\gamma + 1 \mid \frac{2b_\nu r}{Na_0}\right) + (N - \kappa)F\left(-n_r \mid 2\gamma + 1 \mid \frac{2b_\nu r}{Na_0}\right) \right\}, \end{aligned} \quad (23)$$

where a_0 is the Bohr radius, \mathcal{N} is a normalizing constant, $F(a|b|x)$ is a confluent hypergeometric function, and

$$\begin{aligned} N &\equiv \sqrt{n^2 - 2n_r(|\kappa| - \gamma)}, \\ \gamma &\equiv \sqrt{\kappa^2 - \left(\frac{b_\nu e^2}{\hbar c}\right)^2}, \\ n_r &\equiv n - |\kappa|, \\ \mathcal{R} &\equiv \sqrt{\frac{m_0 c^2 - \varepsilon}{m_0 c^2 + \varepsilon}}. \end{aligned} \quad (24)$$

The relativistic energy corresponding to the radial functions shown in equation (23) is

$$\varepsilon = \frac{m_0 c^2}{\sqrt{1 + \left\{ \frac{b_\nu e^2}{\hbar c(\gamma + n_r)} \right\}^2}}. \quad (25)$$

The quantum number n is the principal quantum number familiar to us from our experience with the nonrelativistic hydrogenlike orbitals, and it takes on the values $n = 0, 1, 2, 3, \dots$. The orbital angular momentum quantum number l has the usual

Table 1
Weighting factors b_{n_r} for three basis sets with $j = \frac{1}{2}$ and $l = 0$. All the functions in each set correspond to the same value of ε .

| | | | |
|---------------|---------------|---------------|---------------|
| ε | 0.99572061482 | 0.99728983267 | 0.99848756672 |
| b_0 | 12.6647639832 | 10.0826603634 | 7.53434282976 |
| b_1 | 25.2211331601 | 20.1106693337 | 15.045895277 |
| b_2 | 37.6676916251 | 30.083577687 | 22.5345533075 |
| b_3 | 50.0000000000 | 40.0000000000 | 30.0000000000 |
| b_4 | 62.2099564180 | 49.8574937157 | 37.4416906033 |
| b_5 | 74.2844763552 | 59.6523291207 | 44.8588257443 |
| b_6 | 86.202914867 | 69.3790953363 | 52.2503095934 |

range, $l = 0, 1, 2, \dots, (n - 1)$, while j takes on the values $j = l \pm \frac{1}{2}$ and $m = j, j - 1, \dots, -j$. If we hold b_ν constant while allowing the quantum numbers to vary over their allowed ranges, the resulting set of functions are a set of solutions to the Dirac equation for an electron moving in the attractive potential of a nucleus with charge $b_\nu e$. On the other hand, if we instead pick a constant value of the relativistic energy ε and adjust b_ν so that all the functions in the set correspond to the same energy, regardless of their quantum numbers; and if we normalize the functions so that

$$\int dx \chi_\nu^\dagger(\mathbf{x}) \chi_\nu(\mathbf{x}) \frac{e^2}{r} = \frac{\varepsilon}{b_\nu}, \quad (26)$$

then we will have constructed a one-electron relativistic Coulomb Sturmian basis set. Having chosen a value of ε to characterize one of our basis sets, we must then find the values of b_ν to use as effective nuclear charges in equations (23) and (24). For this purpose it is convenient to use the relationship

$$b_\nu \equiv \frac{137.0429}{a} \left(n_r \sqrt{1 - a} + \sqrt{a\kappa^2 - n_r^2} \right),$$

$$a_\nu \equiv \frac{1}{1 - [\varepsilon/(m_0 c^2)]^2}, \quad (27)$$

which is the inverse of equation (25). Some values of ε are shown in table 1, together with the corresponding values of b_ν . Each basis set constructed in this way was normalized according to the requirements of equation (6), and the normalizing constants are shown in table 2. We verified by numerical integration that within each basis set, the functions corresponding to different b_ν values obey the potential-weighted orthogonality relation. Having constructed Sturmian basis sets of this kind, we can use them to solve the Dirac equation for electrons moving in non-Coulomb potentials.

Table 2
Normalization constants \mathcal{N}_{n_r} for the three basis sets shown in table 1.

| | | | |
|-----------------|---------------|---------------|---------------|
| ε | 0.99572061482 | 0.99728983267 | 0.99848756672 |
| \mathcal{N}_0 | 3.50490397847 | 3.14676040176 | 2.73227902282 |
| \mathcal{N}_1 | 3.38046852466 | 3.08129581173 | 2.70400384175 |
| \mathcal{N}_2 | 3.15988841914 | 2.96220246787 | 2.65125778544 |
| \mathcal{N}_3 | 2.84660243893 | 2.78737637375 | 2.57167470588 |
| \mathcal{N}_4 | 2.45598922690 | 2.55977179867 | 2.46462700697 |
| \mathcal{N}_5 | 2.01290008196 | 2.28654577936 | 2.33084446657 |
| \mathcal{N}_6 | 1.54887618541 | 1.97844726829 | 2.17225843996 |

6. An illustrative example

As a simple illustrative example, we can consider the case of an electron moving in a screened Coulomb potential of the form

$$V(r) = e^2 \frac{Ze^{-r}}{r}. \quad (28)$$

We would like to find the relativistic wave functions and energies for this potential for various values of the nuclear charge Z . The Dirac equation for an electron moving in the potential $V(r)$ is

$$\left[-i\hbar c \boldsymbol{\alpha} \cdot \frac{\partial}{\partial \mathbf{x}} + \gamma_0 m_0 c^2 + V(r) - \varepsilon_\mu \right] \psi_\mu(\mathbf{x}) = 0. \quad (29)$$

In order to solve this equation, we expand the wave function in terms of one of our Sturmian basis sets:

$$\psi_\mu(\mathbf{x}) = \sum_\nu \chi_\nu(\mathbf{x}) C_{\nu,\mu}. \quad (30)$$

Substituting (30) into (29), we obtain

$$\sum_\nu \left[-i\hbar c \boldsymbol{\alpha} \cdot \frac{\partial}{\partial \mathbf{x}} + \gamma_0 m_0 c^2 + V(r) - \varepsilon_\mu \right] \chi_\nu(\mathbf{x}) C_{\nu,\mu} = 0. \quad (31)$$

If $\varepsilon_\mu = \varepsilon$, then, making use of equation (1), we obtain

$$\sum_\nu \left[-b_\nu \frac{e^2}{r} + V(r) \right] \chi_\nu(\mathbf{x}) C_{\nu,\mu} = 0. \quad (32)$$

If we multiply (32) on the left by the adjoint function, $\chi_{\nu'}^\dagger(\mathbf{x})$ and integrate over the coordinates, making use of the potential-weighted orthonormality relations, (6),

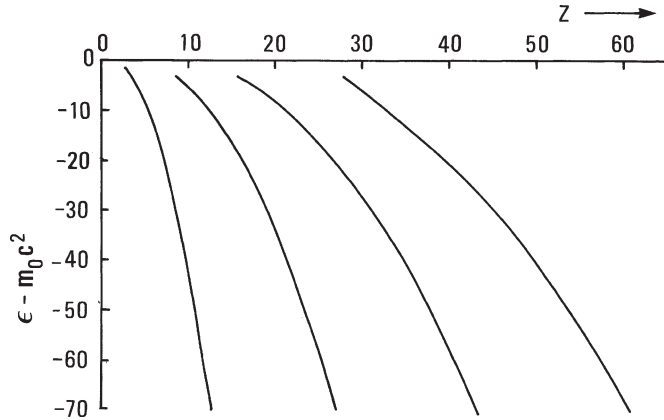


Figure 1. This figure shows the energies of the ground state and the first few excited states with $j = \frac{1}{2}$ and $l = 0$ for an electron moving in the screened Coulomb potential of equation (28). The relativistic energies, from which the electron's rest energy has been subtracted, are expressed in Hartrees, and they are shown as functions of Z .

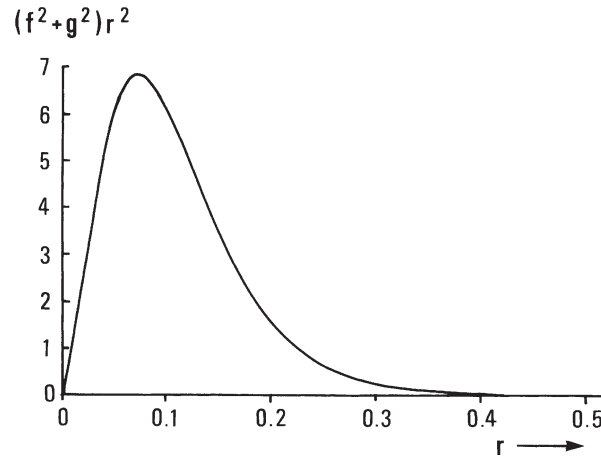


Figure 2. This figure shows the radial distribution function, $[g(r)^2 + f(r)^2]r^2$, for the ground state of an electron moving in a screened Coulomb potential (equation (28)). The solution was obtained using the basis set shown in the first column of table 1, and it corresponds to $Z = 13.6431026$.

the resulting secular equation has a form from which the kinetic energy term has disappeared, as is characteristic for Sturmian secular equations:

$$\sum_{\nu} [V_{\nu',\nu} - \delta_{\nu'\nu} \epsilon_{\mu}] C_{\nu,\mu} = 0, \tag{33}$$

where

$$V_{\nu',\nu} \equiv \int dx \chi_{\nu'}^{\dagger}(\mathbf{x}) V(r) \chi_{\nu}(\mathbf{x}). \tag{34}$$

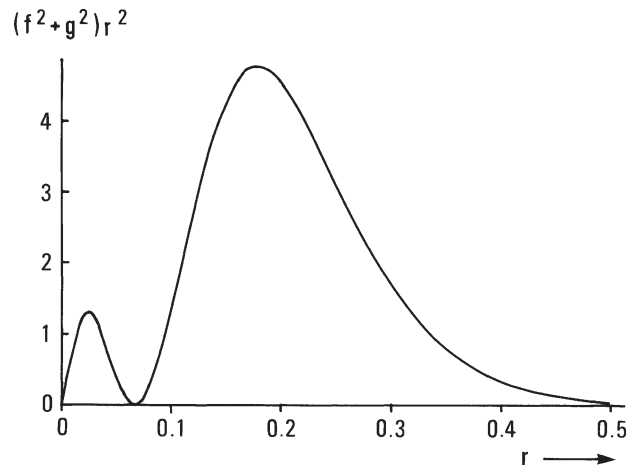


Figure 3. This figure shows the radial distribution function for the first excited state with $j = \frac{1}{2}$ and $l = 0$ for an electron moving in a screened Coulomb potential of the same form. Obtained with the same basis set as that used in figure 2, it corresponds to $Z = 28.9989313$.

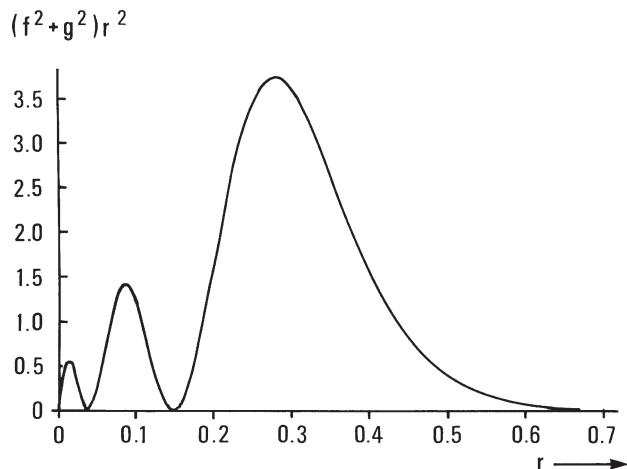


Figure 4. The radial distribution function for the second excited state with $j = \frac{1}{2}$ and $l = 0$ in our illustrative example, again obtained using the same basis set. It corresponds to $Z = 63.9867207$.

Thus the calculation proceeds as follows: We construct matrix elements of $V(r)$ in terms of a basis set characterized by some ε value. We then diagonalize this matrix. For some value of Z , the root corresponding to the ground state will be equal to the ε value characterizing the basis set. This gives us a ground-state solution corresponding to that value of Z . For some other value of Z , the root corresponding to the first excited state will be equal to ε , and so on. If we repeat this procedure using several basis sets, and if we interpolate between the solutions, we can obtain the energies and wave functions as functions of Z , not only for the ground state, but also for the excited states, as illustrated in figures 1–4.

7. Discussion

It is interesting to compare the nonrelativistic concept of Sturmian basis set with the relativistic case. If we continue to use Goscinski's definition [13] rather than Rotenberg's [18], then a nonrelativistic one-electron Sturmian basis set is a set of solutions of the Schrödinger equation for some easily-solved potential $v_0(\mathbf{x})$, where the potential has been weighted by a factor b_ν , especially chosen so that all the functions in the set will have the same energy regardless of their quantum numbers. Thus a member of such a set will satisfy

$$\left[\frac{1}{2}\nabla^2 + E\right]\chi_\nu(\mathbf{x}) = b_\nu v_0(\mathbf{x})\chi_\nu(\mathbf{x}), \quad (35)$$

which is the non-relativistic analogue of equation (1). If we take the complex conjugate of (35) for a different set of quantum numbers, we obtain

$$\left[\frac{1}{2}\nabla^2 + E\right]\chi_{\nu'}^*(\mathbf{x}) = b_{\nu'} v_0(\mathbf{x})\chi_{\nu'}^*(\mathbf{x}), \quad (36)$$

which is the non-relativistic analogue of (3). We now multiply equations (35) and (36) on the left by $\chi_{\nu'}^*(\mathbf{x})$ and $\chi_\nu(\mathbf{x})$, respectively, integrate over the coordinates, and subtract the two equations, making use of the Hermiticity of the operator in square brackets. This yields

$$0 = (b_{\nu'} - b_\nu) \int d\mathbf{x} \chi_{\nu'}^*(\mathbf{x}) v_0(\mathbf{x}) \chi_\nu(\mathbf{x}) \quad (37)$$

from which it follows that functions in the set obey a potential-weighted orthonormality relation. Both in the relativistic case and in the nonrelativistic case, the potential-weighted orthonormality is established by an argument which depends on the Hermiticity of the kinetic energy operator, but which does not require $v_0(\mathbf{x})$ to be a Coulomb potential; nor does the argument for potential-weighted orthonormality require $v_0(\mathbf{x})$ to be spherically symmetric. In fact, in the relativistic case, the "easily solved" potential may have the general form

$$v_0(\mathbf{x}) = e\phi(\mathbf{x}) - e\boldsymbol{\alpha} \cdot \mathbf{A}(\mathbf{x}), \quad (38)$$

where $\phi(\mathbf{x})$ and $\mathbf{A}(\mathbf{x})$ are, respectively, scalar and vector potentials. In the present paper, all of the equations, up to and including equation (15), hold for the general type of potential shown in (38).

In the non-relativistic case, the next step towards generalization is to use the Sturmian expansion of the momentum-space wave equation's kernel to find solutions for an electron moving in a many-center potential. This was first done for the case of many-center Coulomb potentials by Fock, Shibuya and Wulfman [12,19]; and their method has been extended and developed by a number of other authors [3,4,6,7,9,14,15,17]. It is interesting to ask whether an analogous treatment of the one-electron many-center problem can be carried through in the relativistic case; and we hope to explore this question in another paper. We also hope to develop methods for constructing relativistic many-electron Sturmian basis functions analogous to those introduced in the nonrelativistic case by Herschbach, Aquilanti and Avery [2,5,8,10].

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