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## Remarks on completeness of many-electron Sturmians

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**Abstract.** A question of completeness of a discrete many-electron Sturmian set proposed in a series of recent publications is considered. It is shown that already in the simplest case of a two-electron system the proposed Sturmians do not form a complete set since the spectrum of a generating eigenproblem is mixed: apart from discrete eigenvalues, with which the discrete Sturmians are associated as corresponding eigenfunctions, the spectrum also contains a continuum part. A peculiar feature of the spectrum found is that infinitely many discrete eigenvalues are embedded in the continuum.

### 1. Introduction

In the theory of one-electron atomic systems the discrete Coulomb Sturmian functions have been proved to be of particular value (e.g. [1–6] and references therein). It is natural to expect that  $N$ -electron analogues of these functions might be useful in the theory of many-electron atomic systems and, in response to this expectation, over the last decade two different methods of constructing many-electron Coulomb Sturmians have been proposed by Avery, Aquilanti and their collaborators [7–14].

In the first method [7–10], one defines the  $N$ -electron Sturmians as solutions to the Hermitian eigenvalue problem

$$\left[ -\frac{\hbar^2}{2m}\Delta - \mu\frac{Ze^2}{R} \right] \Psi(E, \mathbf{R}) = E\Psi(E, \mathbf{R}) \quad (1)$$

$$R\Psi(E, \mathbf{R}) \xrightarrow{R \rightarrow 0} 0 \quad R^{(3N-1)/2}\Psi(E, \mathbf{R}) \text{ bounded for } R \rightarrow \infty \quad (2)$$

where  $\mathbf{R}$  stands collectively for coordinates of the electrons,  $R$  is the  $N$ -electron hyper-radius defined by

$$R^2 = \sum_{i=1}^N r_i^2 \quad (3)$$

with  $r_i$  denoting the position vector of the  $i$ th electron,  $\Delta$  is a  $3N$ -dimensional Laplace operator,  $m$  and  $e$  are the electron mass and the elementary charge, respectively,  $Z > 0$  and  $E < 0$  are fixed parameters and  $\mu$  is an eigenvalue of the problem. It is known [7–10] that eigensolutions to the problem (1) and (2) form a discrete set which is complete in the space of  $N$ -electron functions. The many-electron Sturmians obtained by solving equations (1) and (2) are currently tested as a basis set in computations of atomic structures [15].

In a recent series of publications [11–14], a method of obtaining an alternative set of many-electron Sturmians has been proposed, namely by solving the Hermitian eigenproblem

$$\left[ -\frac{\hbar^2}{2m} \sum_{i=1}^N \Delta_i - \mu \sum_{i=1}^N \frac{Ze^2}{r_i} \right] \Phi(E, \mathbf{R}) = E \Phi(E, \mathbf{R}) \quad (4)$$

$$r_i \Phi(E, \mathbf{R}) \xrightarrow{r_i \rightarrow 0} 0 \quad r_i \Phi(E, \mathbf{R}) \text{ bounded for } r_i \rightarrow \infty \quad (i = 1, \dots, N) \quad (5)$$

where  $\Delta_i$  is the three-dimensional Laplace operator with respect to coordinates of the  $i$ th electron,  $r_i = |\mathbf{r}_i|$ , the parameters  $m$ ,  $e$ ,  $Z$  and  $E$  are defined as in equation (1) and  $\mu$  is an eigenvalue of the problem. Discrete eigenfunctions of the problem (4) and (5) have been found in [11–14] and applied as a variational basis in exemplary numerical calculations of atomic properties.

If any functional set is to be used as a variational basis in atomic physics or quantum chemistry, the question about its completeness is of extreme importance [16]. Since for the discrete  $N$ -electron Sturmians generated by equations (4) and (5) this problem has not yet been considered, we study it in this paper. For brevity, we restrict our considerations to the simplest but sufficiently representative case of a two-electron atomic system. Utilizing a criterion of completeness of a set of eigenfunctions of a Hermitian differential eigenproblem which states that such a set is complete if it comprises *all* eigenfunctions of the problem, we show that the set proposed in [11–14] is *incomplete* since a spectrum of eigenvalues of the generating eigenproblem is mixed: apart from discrete eigenvalues, with which the proposed Sturmians are associated as corresponding eigenfunctions, the spectrum also contains a continuum of eigenvalues. (A peculiar feature of this spectrum is that infinitely many discrete eigenvalues are embedded in the continuum.) Thus a complete two-electron Sturmian set is formed by eigenfunctions corresponding to discrete eigenvalues *together* with eigenfunctions associated with continuous eigenvalues. Special care is therefore needed when linear combinations of only discrete Sturmians are to be used as trial functions in variational computations.

## 2. The two-electron Sturmians

Consider the eigenvalue problem constituted by the differential equation

$$\left[ -\frac{\hbar^2}{2m} \Delta_1 - \frac{\hbar^2}{2m} \Delta_2 - \mu \frac{Ze^2}{r_1} - \mu \frac{Ze^2}{r_2} \right] \Phi(E; \mathbf{r}_1, \mathbf{r}_2) = E \Phi(E; \mathbf{r}_1, \mathbf{r}_2) \quad (6)$$

augmented by the conditions

$$r_i \Phi(E; \mathbf{r}_1, \mathbf{r}_2) \xrightarrow{r_i \rightarrow 0} 0 \quad r_i \Phi(E; \mathbf{r}_1, \mathbf{r}_2) \text{ bounded for } r_i \rightarrow \infty \quad (i = 1, 2) \quad (7)$$

with fixed parameters  $Z > 0$  and  $E < 0$  and with the parameter  $\mu$  chosen as an eigenvalue. Hermiticity of the eigenproblem guarantees that all its eigenvalues are real.

Equation (6) separates in  $\mathbf{r}_1$  and  $\mathbf{r}_2$ , i.e. it possesses particular product solutions of the form

$$\Phi_{ab}(E; \mathbf{r}_1, \mathbf{r}_2) = \phi_a(E; \mathbf{r}_1) \phi_b(E; \mathbf{r}_2) \quad (8)$$

with single-electron spin-orbitals  $\{\phi_c(E; \mathbf{r})\}$  to be determined. According to [11–14], once a set of solutions (8) to the eigenproblem (6) and (7) is found, the two-electron Schrödinger–Coulomb Sturmian functions are defined as antisymmetrized products of the form

$$\hat{A} \Phi_{ab}(E; \mathbf{r}_1, \mathbf{r}_2) = \phi_a(E; \mathbf{r}_1) \phi_b(E; \mathbf{r}_2) - \phi_b(E; \mathbf{r}_1) \phi_a(E; \mathbf{r}_2) = -\hat{A} \Phi_{ba}(E; \mathbf{r}_1, \mathbf{r}_2). \quad (9)$$

It is clear that if  $\Phi_{ab}(E; \mathbf{r}_1, \mathbf{r}_2)$  is an eigenfunction of (6) and (7) corresponding to the eigenvalue  $\mu_{ab}$ , the Sturmian  $\hat{A}\Phi_{ab}(E; \mathbf{r}_1, \mathbf{r}_2)$  is also an eigenfunction of (6) and (7) corresponding to the same eigenvalue.

To determine the single-electron spin-orbitals, we substitute equation (8) into equation (6). This yields

$$\begin{aligned} \frac{1}{\phi_a(E; \mathbf{r}_1)} \left[ -\frac{\hbar^2}{2m} \Delta_1 - \mu \frac{Ze^2}{r_1} \right] \phi_a(E; \mathbf{r}_1) \\ = -\frac{1}{\phi_b(E; \mathbf{r}_2)} \left[ -\frac{\hbar^2}{2m} \Delta_2 - \mu \frac{Ze^2}{r_2} - E \right] \phi_b(E; \mathbf{r}_2) \end{aligned} \quad (10)$$

and, consequently,

$$\left[ -\frac{\hbar^2}{2m} \Delta_1 - \mu \frac{Ze^2}{r_1} \right] \phi_a(E; \mathbf{r}_1) = E_a \phi_a(E; \mathbf{r}_1) \quad (11a)$$

$$\left[ -\frac{\hbar^2}{2m} \Delta_2 - \mu \frac{Ze^2}{r_2} \right] \phi_b(E; \mathbf{r}_2) = E_b \phi_b(E; \mathbf{r}_2) \quad (11b)$$

where the separation constants  $E_a$  and  $E_b$  are related by

$$E_a + E_b = E < 0. \quad (12)$$

The boundary conditions (7) imply the separated boundary conditions

$$r_1 \phi_a(E; \mathbf{r}_1) \xrightarrow{r_1 \rightarrow 0} 0 \quad r_1 \phi_a(E; \mathbf{r}_1) \text{ bounded for } r_1 \rightarrow \infty \quad (13a)$$

$$r_2 \phi_b(E; \mathbf{r}_2) \xrightarrow{r_2 \rightarrow 0} 0 \quad r_2 \phi_b(E; \mathbf{r}_2) \text{ bounded for } r_2 \rightarrow \infty. \quad (13b)$$

In further considerations it is useful to employ spherical systems of coordinates for  $\mathbf{r}_1$  and  $\mathbf{r}_2$  (though it should be mentioned that spatial parabolic or elliptic coordinates might be used as well) and separate out angular and spin variables, seeking solutions to equations (11a) and (11b) in the forms

$$\phi_a(E; \mathbf{r}_1) = \frac{1}{r_1} P_{l_a}(E; r_1) Y_{l_a m_{l_a}}(\hat{\mathbf{r}}_1) \chi_{\frac{1}{2} m_{s_a}}(1) \quad (14a)$$

$$\phi_b(E; \mathbf{r}_2) = \frac{1}{r_2} P_{l_b}(E; r_2) Y_{l_b m_{l_b}}(\hat{\mathbf{r}}_2) \chi_{\frac{1}{2} m_{s_b}}(2) \quad (14b)$$

where  $\{Y_{lm_l}(\hat{\mathbf{r}})\}$  are spherical harmonics and  $\{\chi_{\frac{1}{2} m_s}\}$  are electron spin eigenfunctions. The radial functions  $P_{l_a}(E; r_1)$  and  $P_{l_b}(E; r_2)$  obey the ordinary second-order equations

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dr_1^2} + \frac{\hbar^2}{2m} \frac{l_a(l_a + 1)}{r_1^2} - \mu \frac{Ze^2}{r_1} \right] P_{l_a}(E; r_1) = E_a P_{l_a}(E; r_1) \quad (15a)$$

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dr_2^2} + \frac{\hbar^2}{2m} \frac{l_b(l_b + 1)}{r_2^2} - \mu \frac{Ze^2}{r_2} \right] P_{l_b}(E; r_2) = E_b P_{l_b}(E; r_2) \quad (15b)$$

where the parameters  $\mu$ ,  $E_a$  and  $E_b$  should be adjusted so that the boundary conditions

$$P_{l_a}(E; r_1) \xrightarrow{r_1 \rightarrow 0} 0 \quad P_{l_a}(E; r_1) \text{ bounded for } r_1 \rightarrow \infty \quad (16a)$$

$$P_{l_b}(E; r_2) \xrightarrow{r_2 \rightarrow 0} 0 \quad P_{l_b}(E; r_2) \text{ bounded for } r_2 \rightarrow \infty \quad (16b)$$

and the constraint (12) are satisfied. We shall achieve this goal within two steps: (a) considering  $\mu$  as a *fixed* parameter and the separation constants  $E_a$  and  $E_b$  as adjustable quantities, we find such values of the latter that corresponding solutions to the system (15a) and (15b) obey the boundary conditions (16a) and (16b); (b) since  $E_a$  and  $E_b$  determined in that way are functions of  $\mu$  and, in general, do not obey (12), in the second step we adjust  $\mu$  so that the latter constraint is satisfied.

To proceed further, we have to consider the cases  $\mu \leq 0$  and  $\mu > 0$  separately.

### 2.1. The case $\mu \leq 0$

In this case equations (15a)–(16b) constitute either radial free-particle problems (if  $\mu = 0$ ) or radial repulsive Coulomb problems (if  $\mu < 0$ ). In either case admissible values of the separation constants are continuous and given by

$$E_a > 0 \quad E_b > 0. \quad (17)$$

Since both are positive, it is clear that there exists no such  $\mu \leq 0$  that the constraint (12) is satisfied. Consequently, there are no non-positive eigenvalues to the problem (6) and (7).

### 2.2. The case $\mu > 0$

In this case equations (15a)–(16b) constitute radial attractive Coulomb problems. Therefore, spectra of the separation constants are mixed, i.e. they contain both discrete and continuous parts, and are given by

$$E_a \in \left\{ -\frac{\mu^2 Z^2 e^2}{2(n_a + l_a + 1)^2 a_0} \right\}_{n_a=0,1,2,\dots} \cup [0, \infty) \quad (18a)$$

$$E_b \in \left\{ -\frac{\mu^2 Z^2 e^2}{2(n_b + l_b + 1)^2 a_0} \right\}_{n_b=0,1,2,\dots} \cup [0, \infty) \quad (18b)$$

where  $n_a$  and  $n_b$  are radial quantum numbers and  $a_0 = \hbar^2/m_e^2$  is the Bohr radius. To determine the spectrum of  $\mu$  we have to consider separately four subcases: (a)  $E_a < 0$  and  $E_b < 0$ , (b)  $E_a < 0$  and  $E_b \geq 0$ , (c)  $E_a \geq 0$  and  $E_b < 0$ , (d)  $E_a \geq 0$  and  $E_b \geq 0$ . The complete spectrum will be the union of the spectra resulting in each of these subcases.

#### 2.2.1. The subcase $E_a < 0$ and $E_b < 0$ . We have

$$E_{n_a l_a} = -\frac{\mu^2 Z^2 e^2}{2N_a^2 a_0} \quad E_{n_b l_b} = -\frac{\mu^2 Z^2 e^2}{2N_b^2 a_0} \quad (19)$$

where

$$N_a = n_a + l_a + 1 \quad N_b = n_b + l_b + 1 \quad (20)$$

are the principal quantum numbers. Substituting equations (19) into the constraint (12) gives the equation for  $\mu$ :

$$-\frac{\mu^2 Z^2 e^2}{2N_a^2 a_0} - \frac{\mu^2 Z^2 e^2}{2N_b^2 a_0} = E. \quad (21)$$

Since  $\mu > 0$ , the solution to equation (21) is

$$\mu_{n_a l_a, n_b l_b} = \frac{K a_0}{Z} \frac{N_a N_b}{\sqrt{N_a^2 + N_b^2}} \quad (22)$$

where

$$K = \sqrt{\frac{2m(-E)}{\hbar^2}}. \tag{23}$$

Substituting back equation (22) into equation (19) gives the final values of the separation constants

$$E_a \equiv E_{n_a l_a, n_b l_b} = \frac{N_b^2}{N_a^2 + N_b^2} E \quad E_b \equiv E_{n_b l_b, n_a l_a} = \frac{N_a^2}{N_a^2 + N_b^2} E. \tag{24}$$

The corresponding radial eigenfunctions are

$$P_{n_a l_a, n_b l_b}(E; r_1) = C_{n_a l_a, n_b l_b} r_1^{l_a+1} \exp(-k_{n_a l_a, n_b l_b} r_1) L_{n_a}^{(2l_a+1)}(2k_{n_a l_a, n_b l_b} r_1) \tag{25a}$$

$$P_{n_b l_b, n_a l_a}(E; r_2) = C_{n_b l_b, n_a l_a} r_2^{l_b+1} \exp(-k_{n_b l_b, n_a l_a} r_2) L_{n_b}^{(2l_b+1)}(2k_{n_b l_b, n_a l_a} r_2) \tag{25b}$$

where  $C_{n_a l_a, n_b l_b}$  and  $C_{n_b l_b, n_a l_a}$  are normalization constants,  $L_n^{(2l+1)}(\rho)$  is the generalized Laguerre polynomial and

$$k_{n_a l_a, n_b l_b} = \sqrt{\frac{2m(-E_{n_a l_a, n_b l_b})}{\hbar^2}} \quad k_{n_b l_b, n_a l_a} = \sqrt{\frac{2m(-E_{n_b l_b, n_a l_a})}{\hbar^2}}. \tag{26}$$

2.2.2. The subcase  $E_a < 0$  and  $E_b \geq 0$ . Then we have

$$-\frac{\mu^2 Z^2 e^2}{2N_a^2 a_0} + E_b = E \quad (E_b \geq 0) \tag{27}$$

hence

$$\mu_{n_a l_a, E_b l_b} = \frac{k_a a_0}{Z} N_a \tag{28}$$

where

$$k_a = \sqrt{\frac{2m(-E_a)}{\hbar^2}} = \sqrt{\frac{2m(E_b - E)}{\hbar^2}} \tag{29}$$

and the principal quantum number  $N_a$  has been defined by equation (20). Since  $E_b$  varies continuously and since the minimal value of  $k_a$ , attained at  $E_b = 0$ , is  $K$  (cf equation (23)), the eigenvalue  $\mu_{n_a l_a, E_b l_b}$  is also continuous and lies in the range

$$\frac{K a_0}{Z} (l_a + 1) \leq \mu_{n_a l_a, E_b l_b} < \infty. \tag{30}$$

The corresponding radial eigenfunctions are

$$P_{n_a l_a, E_b l_b}(E; r_1) = C_{n_a l_a, E_b l_b} r_1^{l_a+1} \exp(-k_a r_1) L_{n_a}^{(2l_a+1)}(2k_a r_1) \tag{31a}$$

$$P_{E_b l_b, n_a l_a}(E; r_2) = C_{E_b l_b, n_a l_a} M_{-i\eta_{ba}, l_b+1/2}(2i\kappa_b r_2) \tag{31b}$$

where

$$\eta_{ba} = \frac{\mu_{n_a l_a, E_b l_b} Z}{\kappa_b a_0} = \frac{k_a}{\kappa_b} N_a \quad \kappa_b = \sqrt{\frac{2mE_b}{\hbar^2}} \tag{32}$$

and  $M_{\eta\gamma}(z)$  is the Whittaker function of the first kind.

2.2.3. *The subcase  $E_a \geq 0$  and  $E_b < 0$ .* This subcase is completely analogous to the preceding subcase. Thus, we have the continuum of eigenvalues

$$\mu_{E_a l_a, n_b l_b} = \frac{k_b a_0}{Z} N_b \quad (33)$$

where

$$k_b = \sqrt{\frac{2m(-E_b)}{\hbar^2}} = \sqrt{\frac{2m(E_a - E)}{\hbar^2}} \quad (E_a \geq 0) \quad (34)$$

in the range

$$\frac{K a_0}{Z} (l_b + 1) \leq \mu_{E_a l_a, n_b l_b} < \infty. \quad (35)$$

The corresponding radial eigenfunctions are

$$P_{E_a l_a, n_b l_b}(E; r_1) = C_{E_a l_a, n_b l_b} M_{-i\eta_{ab}, l_a + 1/2}(2i\kappa_a r_1) \quad (36a)$$

$$P_{n_b l_b, E_a l_a}(E; r_2) = C_{n_b l_b, E_a l_a} r_2^{l_b + 1} \exp(-k_b r_2) L_{n_b}^{(2l_b + 1)}(2k_b r_2) \quad (36b)$$

where

$$\eta_{ab} = \frac{\mu_{E_a l_a, n_b l_b} Z}{\kappa_a a_0} = \frac{k_b}{\kappa_a} N_b \quad \kappa_a = \sqrt{\frac{2mE_a}{\hbar^2}}. \quad (37)$$

2.2.4. *The subcase  $E_a \geq 0$  and  $E_b \geq 0$ .* This subcase is analogous to the case  $\mu \leq 0$  and yields no eigenvalues.

### 3. Discussion

The results obtained in the preceding section may be summarized as follows: the whole spectrum of the problem (6) and (7) consists of discrete positive eigenvalues given by equation (22) with  $N_a \geq 1$  and  $N_b \geq 1$  (note that for  $N_a \rightarrow \infty$  and  $N_b \rightarrow \infty$  one has  $\mu_{n_a l_a, n_b l_b} \rightarrow \infty$ ) and of the continuum covering the range  $[K a_0 / Z, \infty)$ . The discrete eigenvalues in the range  $[K a_0 / \sqrt{2} Z, K a_0 / Z)$  are isolated, while those in the range  $[K a_0 / Z, \infty)$  are embedded in the continuum. The discrete two-electron Sturmian functions are antisymmetric eigenfunctions of the problem (6) and (7) of the form

$$\begin{aligned} \hat{A}\Phi_{n_a l_a m_{l_a} m_{s_a}, n_b l_b m_{l_b} m_{s_b}}(E; \mathbf{r}_1, \mathbf{r}_2) &= \phi_{\{n_a l_a, n_b l_b\} m_{l_a} m_{s_a}}(E; \mathbf{r}_1) \phi_{\{n_b l_b, n_a l_a\} m_{l_b} m_{s_b}}(E; \mathbf{r}_2) \\ &- \phi_{\{n_b l_b, n_a l_a\} m_{l_b} m_{s_b}}(E; \mathbf{r}_1) \phi_{\{n_a l_a, n_b l_b\} m_{l_a} m_{s_a}}(E; \mathbf{r}_2) \end{aligned} \quad (38)$$

where

$$\phi_{\{n_a l_a, n_b l_b\} m_{l_a} m_{s_a}}(E; \mathbf{r}) = \frac{1}{r} P_{n_a l_a, n_b l_b}(E; r) Y_{l_a m_{l_a}}(\hat{\mathbf{r}}) \chi_{\frac{1}{2} m_{s_a}} \quad (39)$$

and similarly for  $\phi_{\{n_b l_b, n_a l_a\} m_{l_b} m_{s_b}}(E; \mathbf{r})$ . In equation (38) the angular momentum and spin quantum numbers run over their usual ranges while the radial quantum numbers  $n_a$  and  $n_b$  run over non-negative integers. The two-electron Sturmians associated with continuous eigenvalues are

$$\begin{aligned} \hat{A}\Phi_{E_a l_a m_{l_a} m_{s_a}, n_b l_b m_{l_b} m_{s_b}}(E; \mathbf{r}_1, \mathbf{r}_2) &= \phi_{\{E_a l_a, n_b l_b\} m_{l_a} m_{s_a}}(E; \mathbf{r}_1) \phi_{\{n_b l_b, E_a l_a\} m_{l_b} m_{s_b}}(E; \mathbf{r}_2) \\ &- \phi_{\{n_b l_b, E_a l_a\} m_{l_b} m_{s_b}}(E; \mathbf{r}_1) \phi_{\{E_a l_a, n_b l_b\} m_{l_a} m_{s_a}}(E; \mathbf{r}_2) \end{aligned} \quad (40)$$

where

$$\phi_{\{E_a l_a, n_b l_b\} m_{l_a} m_{s_a}}(E; \mathbf{r}) = \frac{1}{r} P_{E_a l_a, n_b l_b}(E; r) Y_{l_a m_{l_a}}(\hat{\mathbf{r}}) \chi_{\frac{1}{2} m_{s_a}} \quad (41)$$

and similarly for  $\phi_{\{n_b l_b, E_a l_a\} m_{l_b} m_{s_b}}(E; \mathbf{r})$ . In equation (40) the angular momentum and spin quantum numbers run over their usual ranges, while  $E_a$  runs over real non-negative numbers and  $n_b$  runs over non-negative integers.

Since the discrete Sturmians (38) are associated only with a part of the whole spectrum of the eigenproblem (6) and (7), they do *not* form a complete set in the space of antisymmetric two-electron functions. The complete set, with which converged expansions of arbitrary (i.e. describing either bound or ionized states of a two-electron atom) functions from that space may be obtained, consists of the *totality* of the antisymmetric eigenfunctions (9) to the eigenproblem (6) and (7), i.e. the discrete Sturmians (38) *and* the continuous Sturmians (40).

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