LETTER TO THE EDITOR

Uncoupled correlated calculations of helium isoelectronic bound states

O Chuluunbaatar[1], I V Puzynin[1] and S I Vinitsky[2]

[1] Laboratory of Information Technologies, Joint Institute for Nuclear Research, Dubna, Moscow Region 141980, Russia
[2] Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, Moscow Region 141980, Russia

Abstract

An uncoupled correlated variational method for the calculation of helium isoelectronic bound states is proposed. New projective coordinates $s = r_1 + r_2, v = \frac{r_{12}}{r_1+r_2}, w = \frac{r_1-r_2}{r_{12}}$ are introduced instead of the conventional ones $s = r_1 + r_2, t = r_1 - r_2, u = r_{12}$. All matrix elements of the total Hamiltonian and the weight function are expressed as simple products of three one-dimensional integrals. The variational basis is formed by a set of Laguerre polynomials with a single nonlinear parameter and two sets of Jacobi polynomials for the projective coordinates s, v, w, respectively. It provides a reasonable rate of convergence of the energy, $E = E(N)$, with respect to a number N of the basis components of the eigenvector. The proposed method yields the best available energies for the isoelectronic ground states of the helium atom. New estimations of the isotope helium ground states are also presented.

1. Introduction

In atomic physics uncoupled correlation calculations with a high degree of accuracy have recently been discussed [1]. A variational basis in the special projective coordinates which yield a suitable representation of the overall matrix of the Hamiltonian by simple products of three one-dimensional integrals has been introduced. High accuracy calculations for the ground state of a helium atom with infinite nuclear mass have been carried out. However, this method leads to the Hamiltonian containing δ-function terms and possesses a rather low rate of convergence of the energy $E = E(N)$ versus the number N of terms in the expansion of the eigenvector over the variational basis (so-called 'length N of eigenvector') with a single nonlinear parameter. In particular, the value $E = -2.903\,724\,377\,034\,119\,593\,8(50)$ au has been reported for $N = 8066$ without optimization of the nonlinear parameter [1]. It is interesting to investigate a simpler set of the projective coordinates which provides an uncoupling representation of the matrix elements of the total Hamiltonian and higher rate of convergence of the variational energy.

 In this letter such a set of the projective coordinates is introduced and the corresponding variational basis with a single nonlinear parameter is constructed. The rate of convergence of

the energy of helium isoelectronic ground states is studied and the comparison with known calculations is carried out. As a result, new estimations of the isotope helium ground states are presented.

2. New uncoupled correlated representation

We consider solutions of the Schrödinger equation with the two-electron nonrelativistic Hamiltonian $\overline{H}$ with the nuclear mass being infinite or finite. This Hamiltonian can be rewritten as:

$$\overline{H} = -\frac{1}{2}\left(\nabla_{r_1}^2 + \nabla_{r_2}^2 + \frac{1}{M}\nabla_{r_{12}}^2\right) + \frac{1}{r_{12}} - \frac{Z}{r_1} - \frac{Z}{r_2} \tag{1}$$

where M is the nuclear mass, Z is the nuclear charge, r_i is the distance between the nucleus and the ith electron and r_{12} is the distance between the electrons. In spherical coordinates for two-electron S states the Hamiltonian takes the form

$$\begin{aligned}
H(r_1, r_2, r_{12}) = &-\frac{1}{2}\left(1 + \frac{1}{M}\right)\left(\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1}\right) - \frac{1}{2}\left(1 + \frac{1}{M}\right)\left(\frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2}\right) \\
&-\left(\frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}\right) - \frac{1}{M}\cos\theta\frac{\partial^2}{\partial r_1\partial r_2} + \frac{r_2\cos\theta - r_1}{r_{12}}\frac{\partial^2}{\partial r_1\partial r_{12}} \\
&+\frac{r_1\cos\theta - r_2}{r_{12}}\frac{\partial^2}{\partial r_2\partial r_{12}} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}
\end{aligned} \tag{2}$$

$$\cos\theta = \hat{\mathbf{r}}_1 \cdot \hat{\mathbf{r}}_2 = \frac{r_1^2 + r_2^2 - r_{12}^2}{2r_1 r_2}. \tag{3}$$

The aim of this letter is to present an alternative approach in order to simplify the variational calculations and provide sufficiently higher stability and accuracy. The radial part of the integration volume element can be rewritten in the following way:

$$J = \int_0^\infty r_1\,\mathrm{d}r_1 \int_0^\infty r_2\,\mathrm{d}r_2 \int_{|r_1-r_2|}^{r_1+r_2} r_{12}\,\mathrm{d}r_{12}\, g(r_1, r_2, r_{12}). \tag{4}$$

The three limits of integration are uncoupled by changing the perimetric variables for the new projective coordinates

$$s = r_1 + r_2, \quad v = \frac{r_{12}}{r_1 + r_2}, \quad w = \frac{r_1 - r_2}{r_{12}}. \tag{5}$$

For the new variables (5) the integral (4) is rewritten as

$$I = \int_0^\infty s^5\,\mathrm{d}s \int_0^1 v^2\,\mathrm{d}v \int_0^1 (1 - v^2 w^2)\,\mathrm{d}w\, f(s, v, w). \tag{6}$$

If the function f in the integrand has the form

$$f(s, v, w) = U(s)V(v)W(w) \tag{7}$$

then the integral (6) is fully uncoupled into products of three one-dimensional integrals:

$$I = \int_0^\infty U(s)s^5\,\mathrm{d}s \left\{\int_0^1 V(v)v^2\,\mathrm{d}v \int_0^1 W(w)\,\mathrm{d}w - \int_0^1 V(v)v^4 \int_0^1 W(w)w^2\,\mathrm{d}w\right\}. \tag{8}$$

The full advantage of this decoupling is achieved by choosing the new uncoupled correlated representation for the variational basis set

$$\psi_{i,j,2k} = U_i(s)V_j(v)W_{2k}(w) \tag{9}$$

where $W_{2k}(w)$ are even functions of w for the 1S state of the helium atom. With this basis set all matrix elements of the overlap for the Hamiltonian presented in explicit form [2] can be written as products of one-dimensional integrals (8). The simplest basis functions can be Slater functions for U_i and simple powers for V_j and W_{2k}. Notice that, unlike the case of perimetric coordinates, there is no limitation on the number of the nonlinear parameters which can be introduced for any of the one-dimensional basis functions.

3. Reduction to the algebraic eigenvalue problem

In this work the basis sets used are based on the orthogonal polynomials suited to the domain of integration of each integral. We use

$$U_i(s) = N_i \mathrm{e}^{-\alpha_i s} L_i^5(2\alpha_i s), \quad V_j(v) = \overline{N}_j P_j^{(0,2)}(2v - 1), \quad W_{2k}(w) = \hat{N}_{2k} P_{2k}^{(1,1)}(w) \quad (10)$$

where

$$N_i = \sqrt{\frac{i!(2\alpha_i)^6}{(i+5)!}}, \qquad \overline{N}_j = \sqrt{2j + 3}, \qquad \hat{N}_{2k} = \sqrt{\frac{(k+1)(4k+3)}{2(2k+1)}} \quad (11)$$

are the normalization constants, L_i^5 are the generalized Laguerre polynomials, $P_j^{(q,t)}$ are the Jacobi polynomials and α_i are the variational parameters. By choosing a set with a single parameter α the basis set U_i is orthonormal. With these definitions we have

$$\int_0^\infty s^5 U_n(s) U_m(s) \mathrm{d}s = \delta_{n,m}, \qquad \int_0^1 v^2 V_n(v) V_m(v) \mathrm{d}v = \delta_{n,m},$$

$$\int_0^1 (1 - w^2) W_{2n}(w) W_{2m}(w) \mathrm{d}w = \delta_{2n,2m}. \quad (12)$$

Here the overall overlap matrix consists of a set of block-diagonal arrays, one for each order of the Laguerre polynomials. Using the following additional conditions

$$t = i + a \cdot j + 2b \cdot k \leqslant Nsvw, \qquad d = j + 2k \leqslant Nvw \quad (13)$$

where $Nsvw$ is the largest term in the sum of the orders of U_i, V_j and W_{2k}, Nvw is the largest term in the sum of the orders of V_j and W_{2k} and $a > b > 1$. Now we can find the variational wavefunction in the form

$$\Psi(s, v, w) = \sum_{i,j,k=0}^{t \leqslant Nsvw,\ d \leqslant Nvw} C_{i,j,2k} \psi_{i,j,2k}(s, v, w) \quad (14)$$

where $C_{i,j,2k}$ is the vector of the unknown constants.

After substitution of the expansion (14) into the Rayleigh–Ritz variational functional

$$E(\alpha) = \min_C \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \quad (15)$$

and subsequent minimization of the functional at a fixed value of the nonlinear parameter α, we arrive at an algebraic eigenvalue problem

$$A(\alpha, Z, M)C = E(\alpha)BC. \quad (16)$$

Here $A(\alpha, Z, M) = \alpha^2 A_1(M) + \alpha A_2(Z)$ is the stiffness matrix, B is the mass matrix, $E(\alpha)$ is the eigenvalue and C is the corresponding eigenvector.

We apply the method of inverse iteration with Rayleigh shift to solve the eigenvalue problem (16). Then we use the condition $\partial E(\alpha)/\partial \alpha = 0$ to minimize the energy $E \equiv E(\alpha)$ with respect to the nonlinear parameter α. Table 1 presents different sets of the sizes of

Table 1. Ns, Nv and Nw are the numbers of the one-dimensional basis functions of each type used. N is the total number of components of the eigenvector (14) in the basis set (9)–(10).

Ns	Nv	Nw	$Nsvw$	Nvw	a	b	N
50	14	18	60	18	4.0	2.5	2204
60	14	19	70	19	4.5	2.5	2937
65	14	19	75	19	4.5	2.5	3424
75	15	20	80	20	4.5	2.5	4077
80	15	22	90	22	5.0	3.0	4683
90	15	22	100	22	5.8	3.0	5272
100	15	22	110	22	6.3	3.5	5669

Table 2. Variational parameter values $\alpha \equiv \alpha(Z, N)$ in (10)

N	Z								
	10	9	8	7	6	5	4	3	2
2204	22.0	19.9	17.6	15.4	13.1	10.8	8.6	6.3	3.9
2937	24.8	22.2	19.7	17.2	14.6	12.1	9.6	7.1	4.5
3424	28.1	25.2	22.4	19.5	16.6	13.7	10.9	8.1	5.0
4077	29.2	26.9	23.8	21.2	18.2	15.0	11.9	8.7	5.2
4683	30.5	27.4	24.3	21.2	18.2	15.0	11.9	8.7	5.2
5272	30.5	27.4	24.3	21.2	18.2	15.0	11.9	8.7	5.2
5669	30.5	27.4	24.3	21.2	18.2	15.0	11.9	8.7	5.2

partial bases, in accordance with the resampling down procedure (13), which are finally used to form the N-dimensional ground state vector (14). These sets provide an appropriate condition number of the matrix $A(\alpha, Z, M)$ of the order 10^6, that is three orders better than that for $a = b = 1$ in equation (13). The achieved stability allows one to accelerate the stiffness matrix diagonalization when more than a 13-digit accuracy is required and quadruple-precision calculations are necessary. Note that in real computing we should add a regularization parameter $\varepsilon = 10^{-25}$. Table 2 displays the variational parameter values $\alpha = \alpha(Z, N)$ in au for the set of N values actually used in our calculations. Table 3 shows the variational energy $E = E(N)$ in au and the extrapolation values E^{as} calculated in the present work. The comparison with the other published data is also presented in this table.

4. Comparison of two uncoupled correlation calculations

Below we briefly describe the method of paper [1] to compare it with our approach. In this method the special projective coordinates have been used

$$u = r_>, \qquad v = \frac{r_<}{r_>}, \qquad w = \frac{r_{12} - r_>}{r_<} \tag{17}$$

where $r_> = \max(r_1, r_2)$, $r_< = \min(r_1, r_2)$. The Hamiltonian (2) can be rewritten without trouble in terms of such coordinates

$$r_1 = u(\Theta + v\overline{\Theta}), \qquad r_2 = u(\overline{\Theta} + v\Theta), \qquad r_{12} = u(1 + vw) \tag{18}$$

where Θ is the Heaviside step function

$$\Theta = \Theta(r_1 - r_2) = \begin{cases} 1 & \text{if } r_1 \geqslant r_2 \\ 0 & \text{if } r_1 < r_2 \end{cases} \tag{19}$$

Table 3. Variational energy values $E(N)$ in au, calculated by means of the N-dimensional eigenvector (14) for isoelectronic ($Z = 2, \ldots, 10$) and isotopic (^{4}He and ^{3}He) ground states of helium atoms, in comparison with the data published by other authors. Asymptotic values of energy E^{as} were calculated using the formula (23). The energy values for ^{3}He and ^{4}He are new results for the helium isotopes having nuclear masses $M_{^3He^{2+}} = 5495.8852\, m_e$ and $M_{^4He^{2+}} = 7294.2996\, m_e$ presented in [5].

N	$Z = 10$	$Z = 9$	$Z = 8$	$Z = 7$
2204	−93.906 806 515 037 549 362	−75.531 712 363 959 491 046	−59.156 595 122 757 925 500	−44.781 445 148 772 704 587
2937	−93.906 806 515 037 549 415 2	−75.531 712 363 959 491 098 7	−59.156 595 122 757 925 552 4	−44.781 445 148 772 704 639 1
3424	−93.906 806 515 037 549 419 3	−75.531 712 363 959 491 102 8	−59.156 595 122 757 925 556 4	−44.781 445 148 772 704 643 1
4077	−93.906 806 515 037 549 421 1	−75.531 712 363 959 491 104 5	−59.156 595 122 757 925 558 1	−44.781 445 148 772 704 644 8
4683	−93.906 806 515 037 549 421 372	−75.531 712 363 959 491 104 782	−59.156 595 122 757 925 558 454	−44.781 445 148 772 704 645 091
5272	−93.906 806 515 037 549 421 424	−75.531 712 363 959 491 104 833	−59.156 595 122 757 925 558 506	−44.781 445 148 772 704 645 142
5669	−93.906 806 515 037 549 421 438	−75.531 712 363 959 491 104 847	−59.156 595 122 757 925 558 519	−44.781 445 148 772 704 645 156
E^{as}	−93.906 806 515 037 549 421 453	−75.531 712 363 959 491 104 855	−59.156 595 122 757 925 558 528	−44.781 445 148 772 704 645 162
[6]	−93.906 806 515 037 541			
[7]	−93.906 806 515 037 545 5	−75.531 712 363 959 487 2	−59.156 595 122 757 921 7	−44.781 445 148 772 700 8
[8]	−93.906 806 515 037 4	−75.531 712 363 959 4	−59.156 595 122 757 8	−44.781 445 148 772 6

N	$Z = 6$	$Z = 5$	$Z = 4$	$Z = 3$
2204	−32.406 246 601 898 530 254	−22.030 971 580 242 781 486	−13.655 566 238 423 586 648	−7.279 913 412 669 305 914
2937	−32.406 246 601 898 530 304 6	−22.030 971 580 242 781 535 8	−13.655 566 238 423 586 696 4	−7.279 913 412 669 305 959 5
3424	−32.406 246 601 898 530 308 4	−22.030 971 580 242 781 539 6	−13.655 566 238 423 586 700 0	−7.279 913 412 669 305 962 9
4077	−32.406 246 601 898 530 310 2	−22.030 971 580 242 781 541 3	−13.655 566 238 423 586 701 7	−7.279 913 412 669 305 964 5
4683	−32.406 246 601 898 530 310 464	−22.030 971 580 242 781 541 564	−13.655 566 238 423 586 701 993	−7.279 913 412 669 305 964 836
5272	−32.406 246 601 898 530 310 515	−22.030 971 580 242 781 541 615	−13.655 566 238 423 586 702 043	−7.279 913 412 669 305 964 884
5669	−32.406 246 601 898 530 310 528	−22.030 971 580 242 781 541 627	−13.655 566 238 423 586 702 054	−7.279 913 412 669 305 964 893
E^{as}	−32.406 246 601 898 530 310 535	−22.030 971 580 242 781 541 635	−13.655 566 238 423 586 702 061	−7.279 913 412 669 305 964 899
[6]			−13.655 566 238 423 582	
[7]	−32.406 246 601 898 526 5	−22.030 971 580 242 777 7	−13.655 566 238 423 582 9	−7.279 913 412 669 302 0
[8]	−32.406 246 601 898 4	−22.030 971 580 242 7	−13.655 566 238 423 5	−7.279 913 412 669 2

N	$Z = 2$	^{4}He	^{3}He	
2204	−2.903 724 377 034 119 549	−2.903 304 557 733 234 348	−2.903 167 210 703 584 071	
2937	−2.903 724 377 034 119 593 3	−2.903 304 557 733 234 392 6	−2.903 167 210 703 584 115 5	
3424	−2.903 724 377 034 119 596 3	−2.903 304 557 733 234 395 5	−2.903 167 210 703 584 118 5	
4077	−2.903 724 377 034 119 597 9	−2.903 304 557 733 234 397 2	−2.903 167 210 703 584 120 1	
4683	−2.903 724 377 034 119 598 231	−2.903 304 557 733 234 397 493	−2.903 167 210 703 584 120 433	
5272	−2.903 724 377 034 119 598 280	−2.903 304 557 733 234 397 542	−2.903 167 210 703 584 120 481	
5669	−2.903 724 377 034 119 598 288	−2.903 304 557 733 234 397 550	−2.903 167 210 703 584 120 489	
E^{as}	−2.903 724 377 034 119 598 297	−2.903 304 557 733 234 397 556	−2.903 167 210 703 584 120 495	
[1]	−2.903 724 377 034 119 594			
[3]	−2.903 724 377 034 119 598 296			
[4]	−2.903 724 377 034 119 596			
[6]	−2.903 724 377 034 118			
[7]	−2.903 724 377 034 114			

and $\overline{\Theta} = 1 - \Theta$. However, the corresponding Hamiltonian contains the Dirac delta function

$$\delta(r_1 - r_2) = \frac{1}{u}\delta(1 - v) \tag{20}$$

as has been shown explicitly in [2]. Note that the variables u, v and w have been introduced in the basis set to improve the cusp condition for the probe wavefunction at $r_1 = r_2$ in two ways: (a) by using r_{12} explicitly; (b) by using the variables $r_>$ and $r_<$ [1]. In this case any radial basis function cannot be written as a product of two radial hydrogen-like functions in the coordinates (17)

$$e^{\alpha s} \equiv e^{\alpha(r_1 + r_2)} = e^{\alpha(r_> + r_<)} = e^{\alpha u(1+v)} \tag{21}$$

i.e. it cannot be reduced to the form $f(u)g(v)$ which immediately follows from (10) in accordance with (5). So, if one omits the term uv in the exponent of the right-hand side of equation (21), then the basis set is defined in the form

$$U_i(u) = N_i e^{-\alpha u} L_i^5(2\alpha u), \qquad V_j(v) = \overline{N}_j P_j^{(0,2)}(2v-1), \qquad W_k(w) = \tilde{N}_k P_k^{(0,1)}(w) \tag{22}$$

Table 4. Comparison of the variational energies $E(N)$ in au used with basis vectors (22) and (10) at given values of the charge Z and the variational parameter α.

Z	α^1	α^2	E (au)^1	E (au)^2
10	20.0	28.1	$-93.906\,806\,515\,037\,534$	$-93.906\,806\,515\,037\,549\,419$
9	18.0	25.2	$-75.531\,712\,363\,959\,479$	$-75.531\,712\,363\,959\,491\,102$
8	16.0	22.4	$-59.156\,595\,122\,757\,914$	$-59.156\,595\,122\,757\,925\,556$
7	13.9	19.5	$-44.781\,445\,148\,772\,693$	$-44.781\,445\,148\,772\,704\,643$
6	11.9	16.6	$-32.406\,246\,601\,898\,519$	$-32.406\,246\,601\,898\,530\,308$
5	9.9	13.7	$-22.030\,971\,580\,242\,771$	$-22.030\,971\,580\,242\,781\,539$
4	7.9	10.8	$-13.655\,566\,238\,423\,577$	$-13.655\,566\,238\,423\,586\,700$
3	5.9	8.1	$-7.279\,913\,412\,669\,298$	$-7.279\,913\,412\,669\,305\,962$
2	3.5	5.0	$-2.903\,724\,377\,034\,118$	$-2.903\,724\,377\,034\,119\,596$

^{1} Our results used in the basis vectors (22) for $N = 3795$.
^{2} Our results used in the basis vectors (10) for $N = 3424$.

Table 5. The set of parameters of extrapolation formula (25) at given Z: β is the power of the convergence rate; D_{18} is the constant used for reducing the scale of the energy. ^{4}He and ^{3}He denote the sets for the helium atom isotopes, G is the set for the results of [1].

Z	β	D_{18}
10	≈ 11	$93.906\,806\,515\,037\,549\,421$
9	≈ 11	$75.531\,712\,363\,959\,491\,104$
8	≈ 11	$59.156\,595\,122\,757\,925\,558$
7	≈ 11	$44.781\,445\,148\,772\,704\,644$
6	≈ 11	$32.406\,246\,601\,898\,530\,310$
5	≈ 11	$22.030\,971\,580\,242\,781\,541$
4	≈ 11	$13.655\,566\,238\,423\,586\,701$
3	≈ 11	$7.279\,913\,412\,669\,305\,964$
2	≈ 11	$2.903\,724\,377\,034\,119\,598$
^{4}He	≈ 11	$2.903\,304\,557\,733\,234\,397$
^{3}He	≈ 11	$2.903\,167\,210\,703\,584\,120$
G	≈ 9	$2.903\,724\,377\,034\,119$

where N_i and $\overline{N}_j$ are given by (11), and

$$\tilde{N}_k = \sqrt{\frac{k+1}{2}}.$$

Table 4 shows the corresponding results of our calculation for the variational energy $E(N)$ with the basis vectors (22) and (10) for similar N to compare the convergence rate of the two methods mentioned above. We also studied the extrapolation of such eigenvalues by the formula

$$E^{\text{as}} = E(N) + CN^{-\beta}. \tag{23}$$

We have calculated the values of E^{as}, C, β by minimizing the functional

$$\Phi(E^{\text{as}}, C, \beta) = \sum_{i=1}^{m} \left(\frac{E^{\text{as}} - E(n_i) - Cn_i^{-\beta}}{\delta_i} \right)^2 \tag{24}$$

where δ_i are the calculation errors. The asymptotic values of energy E^{as} are given in table 3 and the corresponding values of the parameter β that show the convergence rate are presented
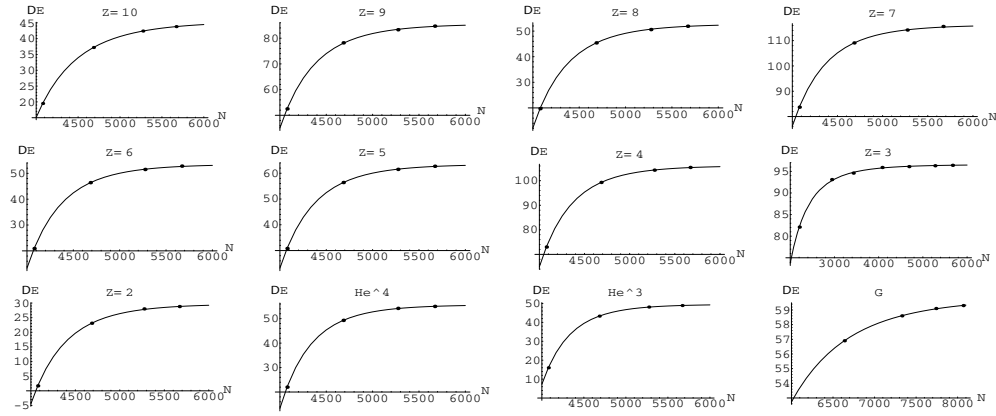
Figure 1. Extrapolation function DE versus N (25) for the ground state energy points $DE(N) = -E(N) - D_{18}$ calculated in this work by means of the N-dimensional eigenvector (14) for the isoelectronic ($Z = 2, \ldots, 10$) and isotopic (^{4}He and ^{3}He) sets with infinite and finite masses from table 3, respectively. The plot G of the extrapolation function DE is restored using the results of the ground state energy [1] for $Z = 2$.
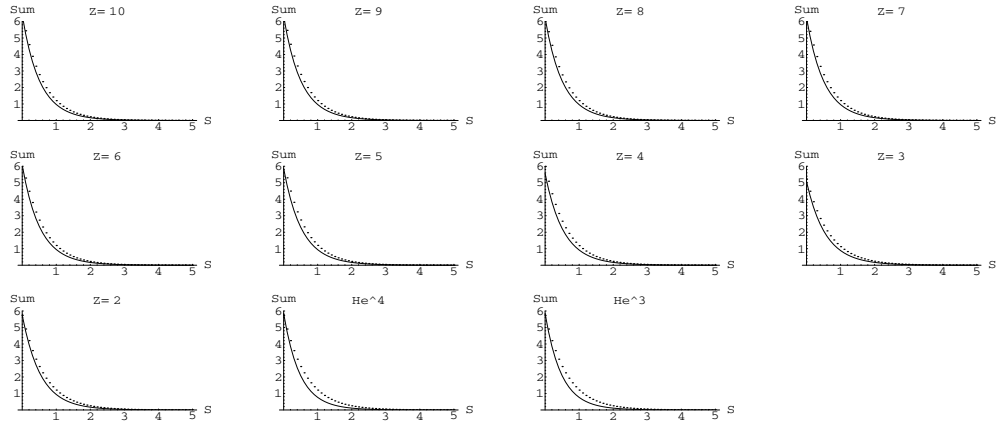

Figure 2. Sum$= \sum C_{i,j,2k} \langle \Psi \rangle_{v,w}$. Dotted curve: radial part of the wavefunction for the basis vectors (10). Full curve: radial part of the wavefunction for the basis vectors (22).

in table 5. It is difficult to display the extrapolation graphically without scaling, so we draw the corresponding plots in figure 1 using the expression

$$DE(N) = \left(-E^{\text{as}} - D_{18} + CN^{-\beta} \right) 10^{20} \tag{25}$$

with the values of D_{18} given in table 5. Finally, we take the basis vectors (22) and (10) to plot the radial parts of the wavefunctions versus s in figure 2 using the above relation (21). One can see that the area under the plots of the radial functions (10) shown by dotted curves is greater than that under the plots of the functions (22) shown by full curves. Table 4 shows that at optimal parameter α found from the condition $\partial E(\alpha)/\partial \alpha = 0$ the convergence rate of the decomposition (10) is better than that given by (22). Evidently, this fact is a consequence of the explicit account for the cusp condition for the coordinate r_{12} in the form (20).

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