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ON UNCOUPLED CORRELATED CALCULATIONS OF HELIUM ISOELECTRONIC BOUND STATES

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1 Introduction

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

In this paper such a set of the projective coordinates is introduced and a corresponding variational basis with a single nonlinear parameter is built up. A study of a degree of convergence of the energy of helium isoelectronic ground states and a comparison with known calculations are undertaken. As result, new estimations of isotope helium ground states are presented.

2 Transformation of conventional nonfactorable variational three-body problem to the factorable one in projective coordinates

We consider solutions of Schrödinger equation with the two-electron nonrelativistic Hamiltonian $\overline{H}$ for an infinite or a finite nuclear mass. Hamiltonian can be rewritten the following way:

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

where M is an infinite or a finite nuclear mass, Z is charge of nuclear, r_i is distance between nuclear and electron, and r_{12} is distance between electrons.

For two-electron S states, in terms of the spherical coordinates the Hamiltonian takes the form

$$H(r_1, r_2, r_{12}) = -\frac{1}{2}\left(1 + \frac{1}{M}\right)\left(\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1} + \frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2}\right) - \left(\frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}\right) -$$

$$-\frac{1}{M}\cos\theta\frac{\partial^2}{\partial r_1 \partial r_2} + \frac{r_2\cos\theta - r_1}{r_{12}}\frac{\partial^2}{\partial r_1 \partial r_{12}} + \frac{r_1\cos\theta - r_2}{r_{12}}\frac{\partial^2}{\partial r_2 \partial r_{12}} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}, \tag{2}$$

$$\cos\theta = \hat{\mathbf{r}}_1 \cdot \hat{\mathbf{r}}_2 = \frac{r_1^2 + r_2^2 - r_{12}^2}{2r_1r_2} \tag{3}$$

The aim of this paper is to present an alternative approach for a simplification of the calculations and providing high stability and accuracy. The radial portion of the integration volume element can be rewritten the following way:

$$J = \int_0^\infty r_1 dr_1 \int_0^\infty r_2 dr_2 \int_{|r_1 - r_2|}^{r_1 + r_2} r_{12} dr_{12} g(r_1, r_2, r_{12}) \tag{4}$$

The three limits of integration are uncoupled by the change of variables

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

The Hamiltonian itself can be easily rewritten in terms of the new coordinates using

$$r_1 = \frac{1}{2}s(1 + vw), \quad r_2 = \frac{1}{2}s(1 - vw), \quad r_{12} = sv. \tag{6}$$

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

$$I = \int_0^\infty s^5 ds \int_0^1 v^2 dv \int_0^1 (1 - v^2w^2) dw f(s, v, w). \tag{7}$$

If the function f in the integrand has the form

$$f(s,v,w) = U(s)V(v)W(w), \tag{8}$$

then the integral (7) is fully uncoupled into products of three one-dimensional integrals:

$$I = \int_0^\infty U(s)s^5 ds \left\{ \int_0^1 V(v)v^2 dv \int_0^1 W(w)dw - \int_0^1 V(v)v^4 \int_0^1 W(w)w^2 dw \right\}. \tag{9}$$

In terms of the new coordinates, the Hamiltonian has the form

$$\begin{aligned} H(s,v,w) = \frac{-1}{s^3 v(1-v^2w^2)} \Bigg\{ & s^3 v \left(1 - v^2w^2 + \frac{2(1-v^2)}{M}\right) \frac{\partial^2}{\partial s^2} + \\ & + sv(1-v^2)\left(1 + v^2w^2 + \frac{2v^2}{M}\right)\frac{\partial^2}{\partial v^2} + s(1-w^2)\left(\frac{1+v^2w^2}{v} + \frac{2v}{M}\right)\frac{\partial^2}{\partial w^2} - \\ & -2s^2v^2(1-v^2)\left(w^2 + \frac{2}{M}\right)\frac{\partial^2}{\partial s \partial v} - 2s^2vw(1-w^2)\frac{\partial^2}{\partial s\partial w} + 4s^2v\left(1+\frac{1}{M}\right)\frac{\partial}{\partial s} + \\ & +2s\left(1 - w^2v^4 - 2v^2 - \frac{2v^4}{M}\right)\frac{\partial}{\partial v} - 2sw\left(\frac{1+v^2}{v} + \frac{2v}{M}\right)\frac{\partial}{\partial w} + s^2(4Zv - 1 + v^2w^2)\Bigg\}. \end{aligned} \tag{10}$$

The Hamiltonian matrix elements can be rewritten as follows:

$$\begin{aligned} <\Psi|H|\Psi> = \int\limits_0^\infty \int\limits_0^1 \int\limits_0^1 \Bigg\{ & s^5v^2\left(1 - v^2w^2 + \frac{2(1-v^2)}{M}\right)\left(\frac{\partial\Psi}{\partial s}\right)^2 + \\ & s^3v^2(1-v^2)\left(1 + v^2w^2 + \frac{2v^2}{M}\right)\left(\frac{\partial\Psi}{\partial v}\right)^2 + \\ & +s^3(1-w^2)\left(1 + v^2w^2 + \frac{2v^2}{M}\right)\left(\frac{\partial\Psi}{\partial w}\right)^2 - \\ & -2s^4v^3(1-v^2)\left(w^2 + \frac{2}{M}\right)\frac{\partial\Psi}{\partial s}\frac{\partial\Psi}{\partial v} - \\ & -2s^4v^2w(1-w^2)\frac{\partial\Psi}{\partial s}\frac{\partial\Psi}{\partial w} - s^4v(4Zv - 1 + v^2w^2)\Psi^2 \Bigg\} dwdvds, \end{aligned} \tag{11}$$

and the matrix element can be rewritten as

$$< \Psi|\Psi >= \int_0^\infty s^5 \int_0^1 v^2 \int_0^1 (1 - v^2w^2)\Psi^2 dwdvds. \tag{12}$$

A full advantage of this decoupling is achieved by choosing a radial basis set of the form

$$\psi_{i,j,2k} = U_i(s)V_j(v)W_{2k}(w), \tag{13}$$

where $W_{2k}(w)$ are even functions for $1S$ state of helium atom. With this basis set, all matrix elements of the overlap for the Hamiltonian can be written as products of one dimensional integrals in the form (9). The simplest basis functions for U_i can be Slater functions and for V_j and W_{2k} simple powers . Notice that, unlike the case of perimeteric coordinates, there is no limitation on the number of nonlinear parameters, which can introduce for any of the one-dimensional basis functions.

3 Reduction of the factorable problem to the algebraic finite generalized eigenvalue problem

In this work the basis sets are based on orthogonal polynomials suited to the domains of integration of each integrals. We use

$$U_i(s) = N_i e^{-\alpha_i s} L_i^5(2\alpha_i s),\ V_j(v) = \overline{N}_j P_j^{(0,2)}(2v - 1),$$
$$W_{2k}(w) = \hat{N}_{2k} P_{2k}^{(1,1)}(w), \tag{14}$$

where

$$N_i = \sqrt{\frac{i!(2\alpha_i)^6}{(i+5)!}},\ \overline{N}_j = \sqrt{2j+3},\ \hat{N}_{2k} = \sqrt{\frac{(k+1)(4k+3)}{2(2k+1)}} \tag{15}$$

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

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

$$\int_0^1 (1 - w^2) W_{2n}(w) W_{2m}(w) dw = \delta_{2n,2m}. \tag{16}$$

Here the overall overlap matrix is made up of a set of block-diagonal arrays, one for each order of the Laguerre polynomials.

Using the following additional conditions

$$\begin{aligned} t = i + a \cdot j + 2b \cdot k \leq Nsvw \\ d = j + 2k \leq Nvw, \end{aligned} \tag{17}$$

where $Nsvw$ is the largest value of terms in the sum of the orders U_i, V_j and W_{2k}, Nvw is the largest value of terms in the sum of the orders V_j and W_{2k}, and $a > b > 1$.

TABLE I. Variational parameter's values α in (14)

Z	10	9	8	7	6	5	4	3	2
α	17.1	15.3	13.6	11.8	10.1	8.3	6.6	5.0	3.0

Now we can write the eigenvector

$$\Psi(s, v, w) = \sum_{i,j,k=0}^{t \leq Nsvw \; d \leq Nvw} C_{i,j,2k} \psi_{i,j,2k}(s, v, w), \tag{18}$$

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

After substitution of expansion (18) in the Rayleigh-Ritz variational functional

$$E(\alpha) = \min_C \frac{< \Psi | H | \Psi >}{< \Psi | \Psi >} \tag{19}$$

TABLE II. Ns, Nv, Nw are the numbers of the one-dimensional basis functions of each type used. N is the total number of vectors in the basis set.

Ns	Nv	Nw	$Nsvw$	Nvw	a	b	N
35	12	16	40	18	3.0	2.0	1175
45	14	18	50	18	3.5	2.5	1561
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

and subsequent minimization of the functional, the solution of (10) is reduced to a solution of a generalized eigenvalue problem for an infinite set.

$$A(\alpha,\ Z,\ M)C = E(\alpha)BC, \tag{20}$$

$$A(\alpha,\ Z,\ M) = \alpha^2 A^1(M) + \alpha A^2(Z) \tag{21}$$

here $A(\alpha,\ Z,\ M)$ is stiffness matrix and B is mass matrix.

An enormous advantage of using orthogonal polynomials for the basis functions are the very high numerical stability of the calculations, which show no sigh of numerical dependence for very large basis set. This stability allows one to accelerate the stiffness matrix diagonalization when more than a 13-digit accuracy is required and quadruple precision calculations are necessary.

TABLE III. Variational energy values E in a.u. obtained in this work and comparison with data published in the literature.
E^{as}Asymptotic values of energy. *New result for the isotopes of helium with $M_{^3He^{2+}} = 5495.8852 m_e$ and $M_{^4He^{2+}} = 7294.2996 m_e$ nuclear mass [2] is presented.

N	$Z = 10$	$Z = 9$	$Z = 8$	$Z = 7$
1175	−93.906 806 515 037 542	−75.531 712 363 959 484	−59.156 595 122 757 918	−44.781 445 148 772 698
1561	−93.906 806 515 037 548 3	−75.531 712 363 959 489 9	−59.156 595 122 757 924 4	−44.781 445 148 772 703 5
2204	−93.906 806 515 037 549 2	−75.531 712 363 959 490 8	−59.156 595 122 757 925 3	−44.781 445 148 772 704 4
2937	−93.906 806 515 037 549 37	−75.531 712 363 959 491 05	−59.156 595 122 757 925 51	−44.781 445 148 772 704 59
3424	−93.906 806 515 037 549 39	−75.531 712 363 959 491 07	−59.156 595 122 757 925 53	−44.781 445 148 772 704 61
4077	−93.906 806 515 037 549 413	−75.531 712 363 959 491 096	−59.156 595 122 757 925 550	−44.781 445 148 772 704 636
4683	−93.906 806 515 037 549 416 6	−75.531 712 363 959 491 099 9	−59.156 595 122 757 925 553 7	−44.781 445 148 772 704 640 2
E^{as}	−93.906 806 515 037 549 423 1	−75.531 712 363 959 491 110 6	−59.156 595 122 757 925 561 5	−44.781 445 148 772 704 648 6
[5]	−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
[6]	−93.906 806 515 037 4	−75.531 712 363 959 4	−59.156 595 122 757 8	−44.781 445 148 772 6
[4]	−93.906 806 515 037 541			

N	$Z = 6$	$Z = 5$	$Z = 4$	$Z = 3$
1175	−32.406 246 601 898 524	−22.030 971 580 242 775	−13.655 566 238 423 581	−7.279 913 412 669 300
1561	−32.406 246 601 898 529 2	−22.030 971 580 242 780 4	−13.655 566 238 423 585 6	−7.279 913 412 669 305 0
2204	−32.406 246 601 898 530 1	−22.030 971 580 242 781 3	−13.655 566 238 423 586 5	−7.279 913 412 669 305 8
2937	−32.406 246 601 898 530 26	−22.030 971 580 242 781 49	−13.655 566 238 423 586 65	−7.279 913 412 669 305 93
3424	−32.406 246 601 898 530 28	−22.030 971 580 242 781 51	−13.655 566 238 423 586 67	−7.279 913 412 669 305 94
4077	−32.406 246 601 898 530 302	−22.030 971 580 242 781 533	−13.655 566 238 423 586 694	−7.279 913 412 669 305 959
4683	−32.406 246 601 898 530 305 8	−22.030 971 580 242 781 536 8	−13.655 566 238 423 586 697 5	−7.279 913 412 669 305 961 5
E^{as}	−32.406 246 601 898 530 311 9	−22.030 971 580 242 781 542 9	−13.655 566 238 423 586 703 9	−7.279 913 412 669 305 966 1
[5]	−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
[6]	−32.406 246 601 898 4	−22.030 971 580 242 7	−13.655 566 238 423 5	−7.279 913 412 669 2
[4]			−13.655 566 238 423 582	

N	$Z = 2$	$(^4He^{2+})^*$	$(^3He^{2+})^*$
1175	−2.903 724 377 034 113	−2.903 304 557 733 228	−2.903 167 210 703 578
1561	−2.903 724 377 034 118 7	−2.903 304 557 733 233 5	−2.903 167 210 703 583 2
2204	−2.903 724 377 034 119 3	−2.903 304 557 733 234 1	−2.903 167 210 703 583 9
2937	−2.903 724 377 034 119 55	−2.903 304 557 733 234 34	−2.903 167 210 703 584 07
3424	−2.903 724 377 034 119 57	−2.903 304 557 733 234 37	−2.903 167 210 703 584 09
4077	−2.903 724 377 034 119 589	−2.903 304 557 733 234 388	−2.903 167 210 703 584 111
4683	−2.903 724 377 034 119 593 3	−2.903 304 557 733 234 392 6	−2.903 167 210 703 584 115 5
5272	−2.903 724 377 034 119 596 3	−2.903 304 557 733 234 395 5	−2.903 167 210 703 584 118 5
5669	−2.903 724 377 034 119 597 4	−2.903 304 557 733 234 396 6	−2.903 167 210 703 584 119 6
E^{as}	−2.903 724 377 034 119 599 9	−2.903 304 557 733 234 398 6	−2.903 167 210 703 584 122 2
[1]	−2.903 724 377 034 119 593 8(50)		
[4]	−2.903 724 377 034 118		
[5]	−2.903 724 377 034 114 4		

We use method Inverse Iteration for calculation eigenvalue. After use to minimize the energy $E \equiv E(\alpha)$ by a nonlinear parameter α

Table I and Table II give variational parameter's values and present the different basis set sizes. Table III shows variational energy values E in a.u. obtained in this work. A comparison with other data published are presented, too.

4 Comparison of the our approach with other factorable variational approach to helium atom in infinite nuclear mass approximation

Below, we describe briefly a method [1] to compare with our approach. In the method [1] the following coordinates are used

$$u = r_>, \; v = \frac{r_<}{r_>}, \; w = \frac{r_{12} - r_>}{r_<}, \tag{22}$$

where $r_> = \max(r_1, r_2), \; r_< = \min(r_1, r_2)$.

The Hamiltonian is rewritten easily in terms of the new coordinates

$$r_1 = u(\Theta + v\overline{\Theta}), \; r_2 = u(\overline{\Theta} + v\Theta), \; r_{12} = u(1 + vw), \tag{23}$$

where Θ is the Heaviside step function

$$\Theta = \Theta(r_1 - r_2) = \begin{cases} 1 & if \quad r_1 \geq r_2 \\ 0 & if \quad r_1 < r_2 \end{cases} \tag{24}$$

and $\overline{\Theta} = 1 - \Theta$.

The new variables u, v and w introduce in the basis set an improvement for the cusp condition for the wave function at $r_1 = r_2$ in two ways: by using r_{12} explicitly as well as by using the variables $r_>$ and $r_<$. The latter, upon substitution in the

Laplacian operators, introduces in the Hamiltonian operator Dirac delta function

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

In terms of the coordinates (22) the Hamiltonian takes the form

$$H(u,v,w) = -\frac{1}{2}\left(1+\frac{1}{M}\right)\frac{\partial^2}{\partial u^2} - \left(\frac{1+v^2}{2u^2} + \frac{(1+vw)^2}{2Mu^2}\right)\frac{\partial^2}{\partial v^2} -$$

$$-\left(\frac{(1+v^2)(1-w^2)}{2u^2v^2(1+vw)} + \frac{(1+vw)(1-w^2)}{2Mu^2v^2}\right)\frac{\partial^2}{\partial w^2} + \left(\frac{v}{u} + \frac{v+2w+vw^2}{2Mu}\right)\frac{\partial^2}{\partial u\partial v} -$$

$$-\left(\frac{(1+v^2)(1-w^2)}{2u^2(1+vw)} + \frac{(1+vw)(1-w^2)}{2Mu^2}\right)\frac{\partial^2}{\partial v\partial w} +$$

$$+\left(\frac{v(1-w^2)}{2u(1+vw)} + \frac{(1-w^2)(2+vw)}{2Muv}\right)\frac{\partial^2}{\partial u\partial w} - \left(\frac{1}{u^2v} + \frac{2-v^2+2vw+v^2w^2}{2Mu^2v}\right)\frac{\partial}{\partial v} -$$

$$-\frac{1}{u}\left(1+\frac{1}{M}\right)\frac{\partial}{\partial u} + \left(\frac{-v+2w+2v^2w+vw^2}{2u^2v^2(1+vw)} + \frac{v+2w+vw^2}{2Mu^2v^2}\right)\frac{\partial}{\partial w} +$$

$$+\left(\frac{1}{u} + \frac{(1+w)^2}{2Mu}\right)\left(\frac{2}{u}\frac{\partial}{\partial v} + \frac{1-w}{u}\frac{\partial}{\partial w} - \frac{\partial}{\partial u}\right)\delta(1-v) - \frac{Z(1+v)}{uv} + \frac{1}{u(1+vw)} \quad (25)$$

The Hamiltonian matrix elements can be rewritten as follows:

$$< \Psi|H|\Psi > = \int_0^\infty\int_0^1\int_{-1}^1 \left\{ u^5v^2(1+vw)\left(1+\frac{1}{M}\right)\left(\frac{\partial\Psi}{\partial u}\right)^2 + \right.$$

$$+u^3v^2(1+vw)\left(1+v^2+\frac{(1+vw)^2}{M}\right)\left(\frac{\partial\Psi}{\partial v}\right)^2 +$$

$$+u^3(1-w^2)\left(1+v^2+\frac{(1+vw)^2}{M}\right)\left(\frac{\partial\Psi}{\partial w}\right)^2 -$$

$$-u^4v^2(1+vw)\left(2v+\frac{v+2w+vw^2}{M}\right)\frac{\partial\Psi}{\partial u}\frac{\partial\Psi}{\partial v} +$$

$$+u^3v^2(1-w^2)\left(1+v^2+\frac{(1+vw)^2}{M}\right)\frac{\partial\Psi}{\partial v}\frac{\partial\Psi}{\partial w} -$$

$$-u^4v(1-w^2)\left(v^2+\frac{(1+vw)(2+vw)}{M}\right)\frac{\partial\Psi}{\partial u}\frac{\partial\Psi}{\partial w} -$$

$$\left. -(2Zu^4v(1+v)(1+vw) - 2u^4v^2)\Psi^2 \right\} dw dv du. \quad (26)$$

TABLE IV. Variational parameter's values α in (28)

Z	10	9	8	7	6	5	4	3	2
α	20.0	18.0	16.0	13.9	11.9	9.9	7.9	5.9	3.5

TABLE V. Comparison variational energy E results in a.u. used with basis vectors (28) and (14).

Z	$E(a.u.)$[1]	$E(a.u.)$[2]
10	−93.906 806 515 037 534	−93.906 806 515 037 549 39
9	−75.531 712 363 959 479	−75.531 712 363 959 491 07
8	−59.156 595 122 757 914	−59.156 595 122 757 925 53
7	−44.781 445 148 772 693	−44.781 445 148 772 704 61
6	−32.406 246 601 898 519	−32.406 246 601 898 530 28
5	−22.030 971 580 242 771	−22.030 971 580 242 781 51
4	−13.655 566 238 423 577	−13.655 566 238 423 586 67
3	−7.279 913 412 669 298	−7.279 913 412 669 305 94
2	−2.903 724 377 034 118	−2.903 724 377 034 119 57

[1] our results used in the basis vectors (28) for N=3795

[2] our results used in the basis vectors (14) for N=3424

The matrix element can be rewritten as

$$< \Psi|\Psi >= 2\int_0^\infty \int_0^1 \int_{-1}^1 u^5 v^2 (1+vw)\Psi^2 dw dv du. \tag{27}$$

Any single radial basis function cannot be written as a product of two radial hydrogenic functions in the coordinates (22)

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

cannot be written as a product of the form $f(u)g(v)$. However, the Taylor expansion of $e^{\alpha u(1+v)}$ is a linear combination of products $f_i(u)g_i(v)$. In the basis set we have

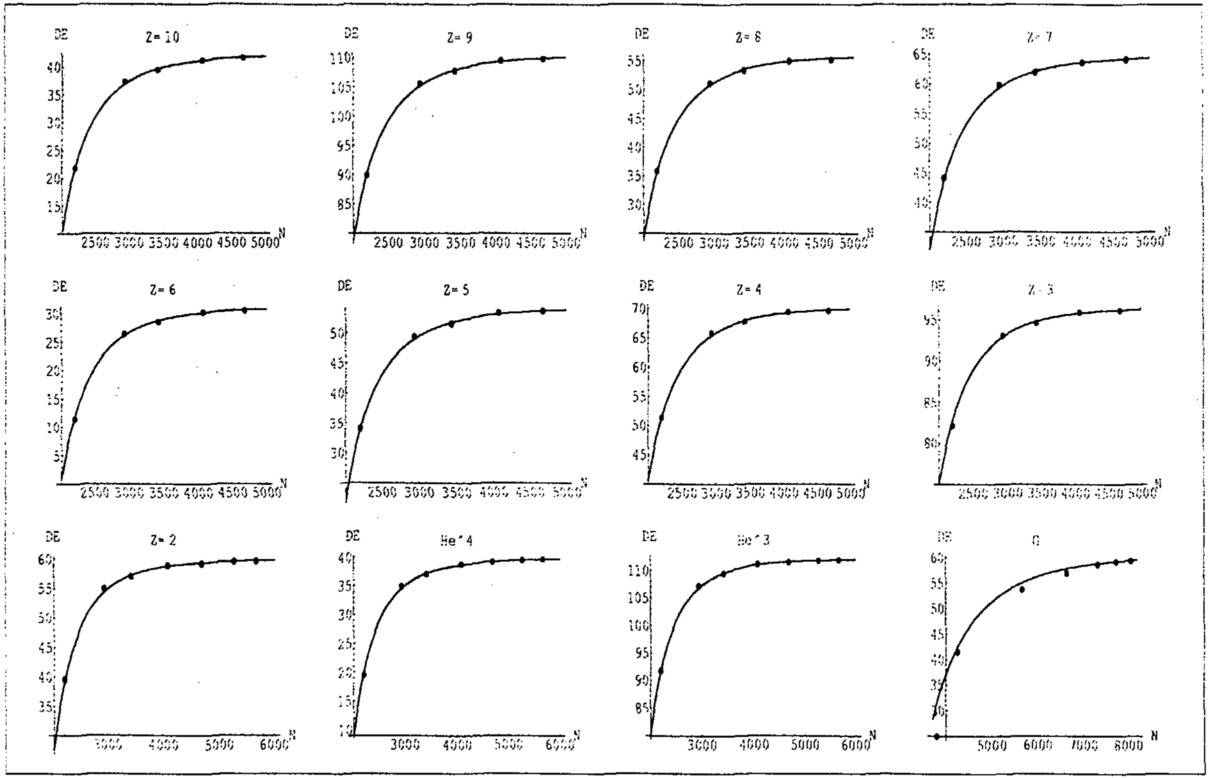

Figure 1: Graphics of extrapolation

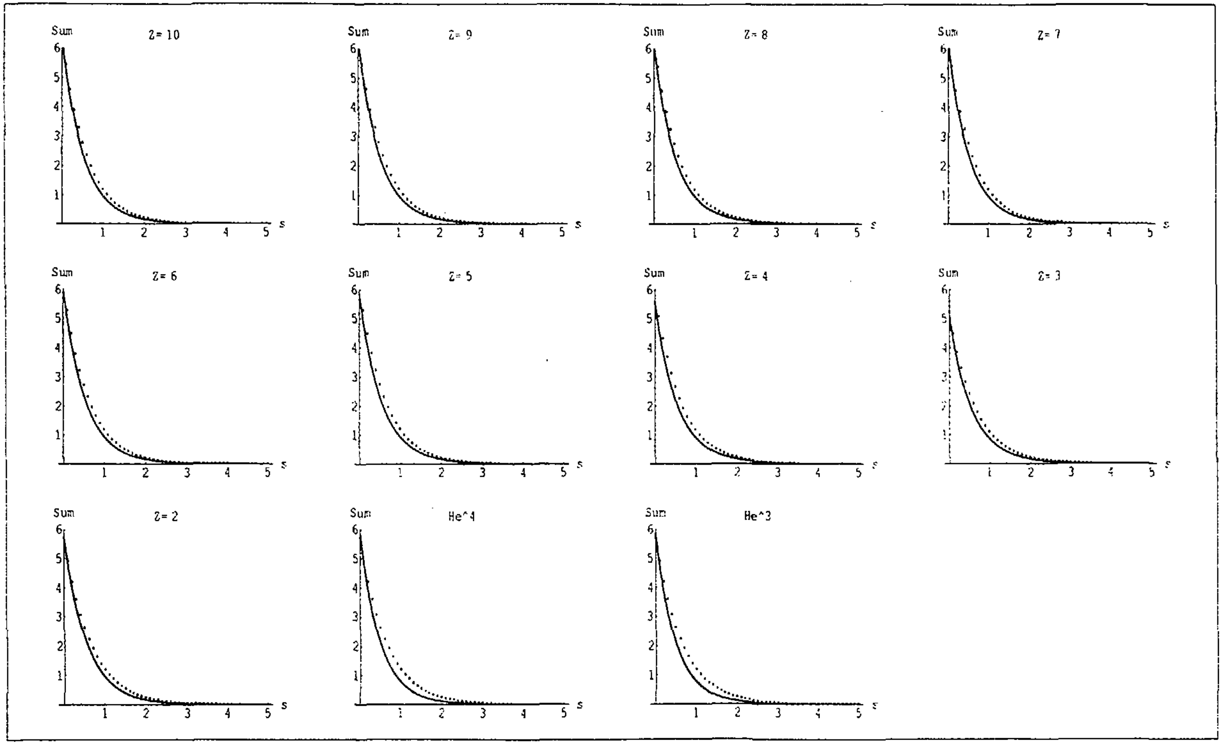

Figure 2. $Sum = \sum C_{i,j,2k} < \Psi >_{v,w}$. Point line: Radial part of wave function for basis vectors (14). Line: Radial part of wave function for basis vectors (28).

$$U_i(u) = N_i e^{-\alpha u} L_i^5(2\alpha u), \quad V_j(v) = \overline{N}_j P_j^{(0,2)}(2v-1)$$

$$W_k(w) = \tilde{N}_k P_k^{(0,1)}(w), \tag{28}$$

where N_i and $\overline{N}_j$ are equal to form (15), and

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

TABLE VI. β is convergence rate; D_{15} is the constant, which is used in the graphic of extrapolation and G is the results of [1]

Z	β	D_{15}
10	4.58	93.906 806 515 037 549
9	4.61	75.531 712 363 959 490
8	4.63	59.156 595 122 757 925
7	4.57	44.781 445 148 772 704
6	4.65	32.406 246 601 898 530
5	4.69	22.030 971 580 242 781
4	4.64	13.655 566 238 423 586
3	4.57	7.279 913 412 669 305
2	4.54	2.903 724 377 034 119
$^4He^{2+}$	4.61	2.903 304 557 733 234
$^3He^{2+}$	4.63	2.903 167 210 703 583
G	4.04	2.903 724 377 034 119

Table IV presents our calculation's result of the variational parameters, used (28). Table V shows corresponded results with basis vectors (28) and (14) for approximate N.

We studied the extrapolation by the formula

$$E^{as} = E(N) + CN^{-\beta}, \tag{29}$$

to compare the convergence rate of the mentioned above two methods. We have solved E^{as}, C, β parameter's values from the conditions minimum of the functional

$$\Phi(E^{as}, C, \beta) = \sum_{i=1}^{m} \left(\frac{E^{as} - E(n_i) - Cn_i^{-\beta}}{\delta_i} \right)^2 , \tag{30}$$

where δ_i error.

One can see the energy asymptotic values from the Table III and the parameter value β, which showed the convergence rate from the Table VI. It is difficult to build the graphics of extrapolation and we built the graphics in Fig. 1, by the formula (see D_{15} from the Table VI)

$$DE = \left(-E^{as} - D_{15} + CN^{-\beta} \right) 10^{17}. \tag{31}$$

In the work, we used the (28) and (14) basis vectors and built the graphics of radial parts of wave functions and showed in Fig. 2.

Here one can see that choosing the optimal parameter α from the condition $\partial E(\alpha)/\partial\alpha = 0$ and the way of solving the energy calculation's rate of convergence by the (14) decomposition is better than the decomposition given in (28).

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