Vol 18 No 6, June 2009
1674-1056/2009/18(06)/2238-06

Chinese Physics B

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Ground state energy of He isoelectronic sequence treated variationally via Hylleraas-like wavefunction*

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(Received 31 July 2008; revised manuscript received 5 September 2008)

In this study, the energy for the ground state of helium and a few helium-like ions (Z=1–6) is computed variationally by using a Hylleraas-like wavefunction. A four-parameters wavefunction, satisfying boundary conditions for coalescence points, is combined with a Hylleraas-like basis set which explicitly incorporates r_{12} interelectronic distance. The main contribution of this work is the introduction of modified correlation terms leading to the definition of integral transforms which provide the calculation of expectation value of energy to be done analytically over single-particle coordinates instead of Hylleraas coordinates.

Keywords: He isoelectronic sequence, Hylleraas basis set, electronic correlation, variational method
PACC: 3130, 3310C

1. Introduction

The theory of two-electron atoms has played an important role in the development of theoretical physics since the early days of quantum mechanics. He and helium-like atoms in which the electron-electron correlation has an important effect, do not have analytical solutions; for this reason these systems have been a field of intensive study since the early days of quantum mechanics.[1,2] Complete understanding of these two-electron systems would guide us to the solution of more complicated many-electron systems. Although several methods have been proposed to solve the problem,[3−6] the variational method is still a standard technique applied in the study of atomic properties.[7−12] The determination of accurate and simple wavefunctions is not only important for the understanding of single-particle properties but also for the understanding of physical processes like double ionization.[10,13,14] The calculation of the cross section of inelastic collision processes involves evaluation of multidimensional integrals.[10] The use of simple wavefunctions allows partial analytical development of double ionization amplitudes which reduces the difficulty of the calculations.[12,13]

Efforts related to the determination of accurate wavefunctions for atomic bound states could be divided into two main approaches: first one is based on sophisticated calculations where many variational parameter wavefunctions are used to produce highly precise approximations.[7,8,15−17] More recently, by using wavefunction depending on exponential-type functions with complex variational parameters chosen in a quasirandom manner, Korobov[17] obtained highly accurate energies for helium and positive hydrogen molecular ion with 2200 number of basis set. Drake[18] used triple basis set in Hylleraas coordinates including 2300 terms and obtained 22-figure accuracy for non-relativistic energy of He. The increment in the number of variational parameters and utilization of huge basis sets needed to improve the wavefunction, generally not only results in more time-consuming calculations,[12] but also it is not realistic for the use in scattering calculations.[19] Within the second approach trial wavefunction generally is constructed to fulfill the correct asymptotic behavior and involves relatively low number of variational parameters.[1,10−12,20,21] Le Sech[10] reported an accuracy for the two-parameter wavefunction which fulfills the cusp conditions at singularities and correct behavior for large interparticle separations to be about 10^{-3}. Patil[11] brought out the structural importance of the correlation property of two-electron systems in terms of simple zero- and one-parameter wavefunc-

*Project supported by the Cumhuriyet University National MOVPE Crystal Growth and Characterization Laboratory, DPT-K 120, TUBITAK (Grant Nos TBAG 105T492, TBAG 107T012, and TBAG-108T015).
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tions. Lateen Ancarani and coworkers[20] proposed the parameter-free simple wavefunction satisfying all two-particle cusp conditions that gave fully analytical expressions for energy and other mean values. The shortage of this approach is that the energies are not good enough to describe the system.[6] Hylleraas-type wavefunctions can be considered as an intermediate approach.[14] After the manifestation of an explicitly correlated basis set at the end of 1920s, several works for the calculation of the ground state energy of He atom and He-isoelectronic sequence using different derivatives of the Hylleraas basis set have been published.[16,17,22–25] Following the method applied by Hylleraas, Schwartz[26] allowed a half-integer powers of the Hylleraas variables while Kinoshita[27] extended the domain of powers of three Hylleraas coordinates to negative integers. After the introduction of the atomic wavefunction closely related to the Hylleraas ansatz by Coolidge and James,[28] successful application of wavefunction depending on perimetric coordinates was done by Pekeris.[15] Frankowski and Pekeris[7] suggested the inclusion of terms with logarithmic dependence.

In this report we focus our work on the determination of ground state energy for helium and He-like ions with nuclear charges $Z = 1 - 6$. A relatively simple wavefunction for obtaining the ground state energy of two-electron atoms is constructed in terms of exponential and power series. In order to fulfill the conditions for the coalescence points special care is taken. Our work, with a low number of parameters, is based on modifying and extending the wavefunction proposed by Bhattacharyya and coworkers[9] with a Hylleraas-like basis set to get better accuracy than the work done by them for He atom and apply the same wavefunction for He-like ions. Variational parameters for improved versions of the ground state wavefunction have been determined. The main contribution of this report is the introduction of the modified correlation term which avoids the use of Hylleraas coordinates. The expectation value of energy is performed by using integral representations that make it possible to carry out the integrations analytically over single-electron coordinates. Atomic units are used throughout this paper.

2. Theory and method

The non-relativistic three-body (two electrons and nucleus) Coulomb Hamiltonian in the infinitely heavy nucleus approximation is given as

$$\hat{H} = -\frac{1}{2}\boldsymbol{\nabla}_{r_1}^2 - \frac{1}{2}\boldsymbol{\nabla}_{r_2}^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}, \qquad (1)$$

where $j = (1, 2)$, r_j, indicates the location of j^{th} electron relative to the nucleus and r_{12} is interelectronic distance. The Hamiltonian (1) includes six independent electronic spherical coordinates. Using a coordinate system which explicitly includes r_{12} interelectronic distance makes it possible to treat the electron-electron correlation effects. The most used is r_1, r_2, r_{12}, α, β and γ basis set where α, β and γ are three Euler angles.[5] After taking away the Euler angles, the Schrödinger equation reduces to the Hylleraas equation which leads to the reduction of the six-dimensional system to the three-dimensional system. For complete description of S-states these three independent coordinates are sufficient.[20,29] Thus the Hamiltonian of the system expressed in Hylleraas coordinates can be written as[30]

$$\hat{H} = -\frac{1}{2}\left(\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1} + \frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}} + 2\hat{\boldsymbol{r}}_1 \cdot \hat{\boldsymbol{r}}_{12}\frac{\partial^2}{\partial r_1 r_{12}}\right)$$

$$-\frac{1}{2}\left(\frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2} + \frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}} - 2\hat{\boldsymbol{r}}_2 \cdot \hat{\boldsymbol{r}}_{12}\frac{\partial^2}{\partial r_2 r_{12}}\right) - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}, \qquad (2)$$

where $\hat{\boldsymbol{r}}_1$, $\hat{\boldsymbol{r}}_2$ stands for the unit vectors for electron-nucleus distance and $\hat{\boldsymbol{r}}_{12}$ denotes the unit vector of interelectronic distance.

One of the most important points in the study of two-electron systems is the choice of wavefunction which satisfies proper symmetry under the interchange

of the electron coordinates and correct cusp conditions that are responsible for the two-body Coulomb singularities. The ground state wavefunctions of He and He-like ions are expressed as a product of wavefunction describing the orbital motion of free-particles in the field of nucleus area and a correlation function depending on the interelectronic distance r_{12}.[9,10] Following these ideas we proposed here in this article wavefunction, without inclusion of the Hylleraas basis set, that ensures the conditions: the separability of the wavefunction when the two electrons are far apart $r_{12} \to \infty$ and requirement of small finite value of correlation function in $r_{12} \to 0$ limits. The wavefunction proposed in this connection is constructed as a product of Slater-type orbitals that are solutions of non-interacting system and $(1 - \lambda e^{-\mu r_{12}})$ term which defines two-electron correlation. Our ansatz for finding the appropriate wavefunction describing the ground state of atom (ions) in He isoelectronic sequence is chosen in the form of

$$\phi(r_1, r_2, r_{12}) = e^{-Z\alpha(r_1+r_2)} e^{-\beta r_{12}} (1 - \lambda e^{-\mu r_{12}}), \quad (3)$$

where α, β, λ and μ are adjustable variational parameters and Z denotes the nuclear charge. The difference between the wavefunction of Bhattacharyya[9] and ours is the $e^{-\beta r_{12}}$ term that is important for the evaluation of integrals by means of integral representations obtained for the terms containing powers of r_{12} coordinates. The approximate solution is built by expanding the wavefunction expressed in analytical form with the Hylleraas-like basis set

$$\Phi(r_1, r_2, r_{12}) = \sum_N C_N \, \Psi^N(r_1, r_2, r_{12}), \quad (4)$$

where

$$\Psi^N(r_1, r_2, r_{12}) = \phi(r_1, r_2, r_{12})(1 + P_{12}) r_1^{n_1} r_2^{n_2} r_{12}^{n_{12}}. \quad (5)$$

Here n_i $(i = 1, 2, 12)$ are integers and $N \equiv \{n_1, n_2, n_{12}\}$ are sets of all parameters incorporated in wavefunction. P_{12} denotes permutation operator of coordinates r_1 and r_2. Factor $(1 + P_{12})$ accounts for spatial symmetric combinations associated with singlet state. For simplicity, in what follows we shall drop the (r_1, r_2, r_{12}) dependence of $\Psi^N(r_1, r_2, r_{12})$. As a consequence of $S = 0$ (antisymmetric spin function) for the ground state of the systems, spatial function Ψ has to be symmetric under the exchange of electron coordinates imposing the constraint $C_{n_1,n_2,n_{12}} = C_{n_2,n_1,n_{12}}$. To fulfill with that symmetry the series on Eq.(4) has to include terms up to the same value of the indices n_1 and n_2. In order to investigate the convergence of each form of a given excitation level all possible combinations of variables have been considered. Optimization with respect to the C_N linear expansion coefficients in Eq.(4) is a generalized eigenvalue problem, consisting in diagonalization of matrix

$$\sum_N [\boldsymbol{H} - E\,\boldsymbol{S}]\, C_N = 0, \quad (6)$$

Here matrix $\boldsymbol{H}$ denotes kinetic energy, energy from Coulomb interaction and interaction with nucleus whereas matrix $\boldsymbol{S}$ denotes the norm with respect to the basis function. C_N stands for column matrix of $C_{n_1,n_2,n_{12}}$ coefficients. Elements of overlap matrix $\boldsymbol{S}$ are given as

$$\begin{aligned} S_{M,N} &= \langle \Psi^M | \Psi^N \rangle \\ &= \iint \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \, \Psi^{M^*} \Psi^N, \end{aligned} \quad (7)$$

and elements of $\boldsymbol{H}$ Hamiltonian matrix are

$$\begin{aligned} H_{M,N} &= \langle \Psi^M | \hat{H} | \Psi^N \rangle \\ &= \frac{1}{2} \iint \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \big(\boldsymbol{\nabla}_{r_1} \Psi^{M^*} \cdot \boldsymbol{\nabla}_{r_1} \Psi^N \\ &\quad + \boldsymbol{\nabla}_{r_2} \Psi^{M^*} \cdot \boldsymbol{\nabla}_{r_2} \Psi^N \big) \\ &\quad - Z \iint \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \, \Psi^{M^*} \left(\frac{1}{r_1} + \frac{1}{r_2} \right) \Psi^N \\ &\quad + \iint \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \, \Psi^{M^*} \frac{1}{r_{12}} \Psi^N. \end{aligned} \quad (8)$$

The general procedure for the evaluation of integrals in order to determine ground state energy while working with wavefunctions expressed in Hylleraas coordinates is using the coordinates $u = r_{12}$, $s = r_1 + r_2$ and $t = r_1 - r_2$. Integrals in type of $I = \int F(r_1, r_2) f(r_{12}) \mathrm{d}^3 r_1 \mathrm{d}^3 r_2$ are expressed in terms of Hylleraas coordinates as $I = 8\pi^2 \int F(r_1, r_2) r_1 \mathrm{d}r_1 r_2 \mathrm{d}r_2 \int f(r_{12}) r_{12} \mathrm{d}r_{12}$ where limits of integration over the r_{12} coordinate are $|r_1 - r_2|$ and $(r_1 + r_2)$.[11]

In this work, unlike the general procedure mentioned above, the Fourier transforms have been used for the terms including r_{12} interelectronic distance[9,31]

$$\frac{e^{-\lambda r}}{r} = \frac{1}{2\pi^2} \int \frac{e^{i\boldsymbol{p}\cdot\boldsymbol{r}}}{(\lambda^2 + p^2)} \mathrm{d}\boldsymbol{p} \quad (9)$$

and

$$\frac{1}{r_{12}} = \frac{1}{2\pi^2} \int \frac{e^{i\boldsymbol{R}\cdot(\boldsymbol{r}_1 - \boldsymbol{r}_2)}}{R^2} \mathrm{d}\boldsymbol{R}. \quad (10)$$

Utilization of these transforms leads to the general integral representations for the terms in the form $e^{-\lambda r_{12}}.r_{12}^k$, ($\lambda$ is parameter and $k \in \boldsymbol{Z}$) which avoid the use of general Hylleraas-like integrations mentioned above. The obtained integral representations are

$$\int d\Omega_1 \int d\Omega_2 \, e^{-\lambda r_{12}}.r_{12}^{(p-1)}$$
$$= 32\pi \int_0^\infty dq \, \frac{\sin(qr_1)}{r_1} \, \frac{\sin(qr_2)}{r_2} \, Q[q,\lambda,p],$$
$$Q[q,\lambda,p] = (-1)^p \frac{\partial^p}{\partial \lambda^p} \left[\frac{1}{(q^2+\lambda^2)} \right],$$
$$p = 0, 1, 2, \ldots \qquad (11)$$

where Ω_i ($i = 1, 2$) are solid angles related to each electron. Since these integral representations separate coordinates of each electron from other one, integrals in similar form are obtained for each electron. These separated integrals are calculated analytically in terms of gamma and trigonometric functions. Integrations over r_1 and r_2 coordinates are performed analytically whereas numerical procedure is applied for the integrations over q variable coming from the integral representations.

3. Results and discussion

We have performed calculations for ground state energy of He atom and He-like ions by means of a wavefunction expressed as a Hylleraas-like basis set (4), which spans powers $\{n_1, n_2, n_{12}\}$ for the corresponding coordinates r_1, r_2 and r_{12} and commensurate with the condition $n_1+n_2+n_{12} \leq 8$. Calculations of ground state energies have been actualized in two stages. The first one is getting α, λ and μ variational parameters which minimizes energy by using Eq.(3), in other words without using a Hylleraas-like series expansion with $\beta \simeq 0$, $n_{1\max} = 0$, $n_{2\max} = 0$ and $n_{12\max} = 0$

Table 1. Ground state energies of H^-, He, Li^+, Be^{2+}, B^{3+}, C^{4+} calculated using the wavefunction given in Eq.(3) and values of the corresponding optimized parameters. All obtained energies are in atomic units.

system	Z	α	λ	μ	–energy
H^-	1	0.81	0.89	0.07	0.5076
He	2	0.92	0.95	0.02	2.8911
Li^+	3	0.94	0.44	0.60	7.2669
Be^{2+}	4	0.96	0.61	0.22	13.6443
B^{3+}	5	0.96	0.22	1.52	22.0167
C^{4+}	6	0.98	0.46	0.45	32.3951

we obtained optimal values of variational parameters. Here the notation $n_{(i)_{\max}}$, where ($i = 1, 2, 12$), indicates the maximum power of corresponding coordinate. Columns three, four and five of Table 1 present the optimized values of variational parameters. The corresponding calculated energies of the systems H^-, He, Li^+, Be^{2+}, B^{3+} and C^{4+} are given at the last column of Table 1.

The second stage of the calculation is incorporating the Hylleraas-like series expansion by using the values of parameters obtained at the first stage. We introduced the exponential factor $e^{-\beta r_{12}}$ in the wavefunction (3) in order to calculate the integrals related to interelectronic distance analytically by using Fourier transforms as in Eqs.(9) and (10). Also we fixed the parameter β to 10^{-2} for all two-electron systems since it showed a little sensitivity to the evaluated energy value. Expansion of different powers, (n_1, n_2, n_{12}), of all coordinates is performed by putting into account the values for non-linear variational parameters obtained in the first stage of the calculation. By using the wavefunction as in Eq.(4), relatively low expansions are sufficient to accomplish reasonably accurate energies describing the ground state of the systems. To illustrate the appreciable improvement on the energy of adding more terms to the expansion, we show the dependency of energy with a different number of maximum degrees of n_1, n_2 and n_{12} only for He atom in Table 2.

Table 2. Ground state energy of He atom (in atomic units) for different number of maximum degrees of n_1, n_2 and n_{12} corresponding to the coordinates r_1, r_2 and r_{12} respectively.

$n_{1\max}(n_{2\max})$	$n_{12\max}$	–energy
1	1	2.8969
2	1	2.9030
3	1	2.9033
1	2	2.9028
2	2	2.9032
3	2	2.9034

Inclusion of higher degrees of r_1, r_2 and r_{12} coordinates into the expansion leads to a considerable improvement in variational energy for the systems considered in this work. This situation is evident in Table 3 in comparison to the energies given in Table 1.

Table 3. Ground state energies calculated using the wavefunction given in Eq.(4) and electron-electron cusp condition. Exact energies are taken from Ref.[32]. All energies are in atomic units.

system	Z	−energy	−energy$_{\text{exact}}$	R_{ee}
H^-	1	0.5268[a]	0.5277	0.5564
		0.5258[b]		
		0.5259[c]		
He	2	2.9034[a]	2.9037	0.3700
		2.9020[b]		
		2.9019[c]		
Li^+	3	7.2797[a]	7.2799	0.4614
		7.2778[b]		
		7.2780[c]		
Be^{2+}	4	13.6551[a]	13.6555	0.3440
		13.6534[b]		
		13.6536[c]		
B^{3+}	5	22.0307[a]	22.0309	0.3781
		22.0287[b]		
		22.0290[c]		
C^{4+}	6	32.4056[a]	32.4062	0.3733
		32.4039[b]		
		32.4043[c]		

[a] this study, [b] Ref.[6], [c]Ref.[12]

The conditions that measure the quality of the approximate wavefunction at singular points of potentials have been tested. Parameters related to the electron-nucleus coalescence point are not far from their exact values. The expected value for this coalescence point is equal to the negative value of nuclear charge of the two-electron system. So in our calculations the value of the non-linear α parameter should be equal to 1. As seen in Table 1 the α parameter approaches to its exact value with increase in nuclear charge. Parameters related to the electron-electron coalescence point, R_{ee}, are presented in Table 3. Except in the case of H^-, obtained values for R_{ee} are smaller than the expected value which is 0.5. This can be interpreted as underestimation of interelectronic repulsion by the proposed wavefunction. But more significantly ground state energies of isoelectronic sequence have been found to be within reasonable accuracy. The wavefunction proposed in this work yields ground-state energies for the helium-like atoms with $Z = 1$ (H^-) to $Z = 6$ (C^{4+}) within 0.0009–0.0002 a.u. of the exact energies of Ref.[32] which is widely used in the literature as a reference work. These results are significantly better than the results obtained with previous models. Rodriguez and coworkers[6] reported angular correlated configuration-interaction method to analyze n-parameter Hylleraas wavefunctions satisfying all cusp conditions. Results obtained by Rodriguez[6] are given in Table 3 for comparison. We also compared energies with the energies found by Otranto and coworkers.[12] They used relatively simple analytical wavefunctions, by modifying the wavefunctions used by Bonham *et al*[33] and Le Sech.[10] In spite of a little complexity, relative to Ref.[12], the wavefunction proposed in this work gave slightly closer values for energy. This can be interpreted thus: the wavefunction proposed in this work describes better the ground state of the systems under consideration.

4. Conclusion

Ground state energies of He-like ions have been calculated via a Hylleraas-like wavefunction. Utilizing minimization parameters obtained from the three-parameter wavefunction, series expansion leads to the significant improvement on the energy. Due to the built-in correlated character of the wavefunction relatively low expansions are sufficient to accomplish reasonable energies. In this work unlike general numerical integration procedure for Hylleraas coordinates, Fourier transforms obtained for $e^{-\lambda r_{12}} r_{12}^p$ terms have been used. Most of integrations have been performed analytically. The inevitable numerical procedure has been invoked at the last stage of calculations. The accuracy for all two-electron systems which have been investigated in this work is better than 1×10^{-3} a.u..

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