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Geometric quantities of lower doubly excited bound states of helium

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Expectation values of single electron and interelectronic geometric quantities such as $\langle r\rangle$, $\langle r_{12}\rangle$, $\langle r_<\rangle$, $\langle r_>\rangle$, $\langle\cos\theta_{12}\rangle$ and $\langle\theta_{12}\rangle$ are calculated for doubly excited $2pnp\,^1P^e$ $(3\le n\le 5)$, $2pnp\,^3P^e$ $(2\le n\le 5)$ and $2pnd\,^{1,3}D^o$ $(3\le n\le 5)$ states of helium using Hylleraas-*B*-spline basis set. The energy levels converge to at least 10 significant digits in our calculations. The extrapolated values of geometric quantities except for $\langle\theta_{12}\rangle$ reach 10 significant digits as well; $\langle\theta_{12}\rangle$ reaches at least 7 significant digits using a multipole expansion approach. Our results provide a precise reference for future research.

Keywords: doubly excited states, unnatural parity, Hylleraas-*B*-spline, geometric quantities

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1. Introduction

The first evidence of existence of doubly excited states (DESs) is the observation of a line of 32.079 nm in the emission spectrum of helium by Comptom and Boyce.[1] Kruger attributed it to the transition between the $2p^2\,^3P^e$ and $1s2p\,^3P^o$ states two years later,[2] and it was confirmed by Wu soon.[3] The existence of DESs of helium has stimulated plenty of research. For example, Hilger *et al.* using the Hylleraas basis presented precise energy levels of $^{1,3}P^e$ states of helium below the second ionization threshold of He^+.[4] Using the complex-rotation method, Ho and Bhatia calculated resonance parameters of $^{1,3}P^e$ and $^{1,3}D^o$ states of helium-like systems below the $N=3$–5 threshold of He^+.[5,6] These $^3P^e$ states were also calculated by Saha and Mukherjee using the stabilization method.[7] However, there are some discrepancies between the results presented by Saha *et al.*[7] and by Hilger *et al.*[4] and Ho *et al.*[5] To make the reason of discrepancies clear, Kar and Ho[8] recalculated resonance parameters of $^3P^e$ states of helium using both complex-rotation method and stabilization method with correlated exponential wavefunctions. Their results are consistent with Hilger *et al.*[4] and Ho *et al.*[5] Using spectral approach, Eilglsperger presented a wide range of energy levels for meta-stable bound states $^{1,3}L$ with total angular momentum $L=1$–9, and of resonance parameters for resonance $^{1,3}P^e$ states below $N=3$–5 threshold of He^+.[9,10]

Besides the resonance parameters, geometric quantities are also important physical quantities describing information of states, such as $\langle r\rangle$, $\langle r_{12}\rangle$, $\langle r_<\rangle$, $\langle r_>\rangle$, $\langle\cos\theta_{12}\rangle$ and $\langle\theta_{12}\rangle$, which represent electron-nucleus radial distance, interelectronic radial distance, radial distance between inner electron and nucleus, radial distance between outer electron and nucleus, cosine of interelectronic angle and interelectronic angle, respectively. The $\langle r_>\rangle$ could be used to estimate the resonance general size and to distinguish the difference resonance states series of H^-.[11,12] In addition, $\langle r_<\rangle$, $\langle r_>\rangle$ and $\langle\cos\theta_{12}\rangle$ could be used to construct the Lewis structures for resonance states.[13] Angular quantities $\langle\theta_{12}\rangle$, $\langle\cos\theta_{12}\rangle$ could be used to study the resonance parameters of plasma-embedded helium.[14] The interference phenomena between difference resonance series could also be described by these geometic quantities.[13] Systemically investigations on expectation values of these geometric quantities for ground and singly excited states of two-electron systems was completed based on the HF and MCHF methods by Koga group,[15–18] and based on full STO-CI framework and Hylleraas-CI method by Jiao.[19,20] Koga *et al.* also pointed out that for singlet and triplet singly excited states, $\langle r\rangle$ and $\langle r_{12}\rangle$ could be fitted into nearly linear law formulas.[18] However, to our best knowledge, the works focusing on geometric quantities of DESs of two-electron systems are relatively rare. In this work, we calculate the geometric quantities of $^{1,3}P^e$ and $^{1,3}D^o$ states of helium based on Hylleraas configuration interaction approach using the Hylleraas-*B*-spline (H-*B*-spline) basis. These states are doubly excited, which indicates that the wavefunctions distribute in a wider radial range. The variational basis should have good fitting abilities. On another hand, precise calculations on lower lying states needs large partial-wave expansion. Recently, Yang *et al.* introduced a convenient basis set, called the H-*B*-spline basis, by integrating the $r_{12}=|\boldsymbol{r}_1-\boldsymbol{r}_2|$ factor in the *B*-spline basis.[21] This basis inherits the virtue of traditional *B*-spline basis, the high localization of each spline, and also has the ability of describing the behavior of wavefunctions at two-electron coalescences, which improves greatly the rate of convergence in partial-wave expansion. The H-*B*-spline basis was successfully applied to

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calculation on polarizabilities, magic wavelengths and Bethe logarithm of helium.[21–23] Here we will use this basis to calculate DESs, $2pnp\,^1P^e\,(3\le n\le 5)$, $2pnp\,^3P^e\,(2\le n\le 5)$ and $2pnd\,^{1,3}D^o\,(3\le n\le 5)$, of helium.

This article is organized as follows. Section 2 includes a brief introduction of the H-*B*-spline basis and the computational methodology in calculating geometric quantities. Convergence studies of energy levels and geometric quantities of $2pnp\,^1P^e\,(3\le n\le 5)$, $2pnp\,^3P^e\,(2\le n\le 5)$ and $2pnd\,^{1,3}D^o\,(3\le n\le 5)$ states are presented in Section 3. Discussion are made in this section as well. Finally, a summary is given in Section 4. Atomic units are used throughout this article.

2. Theoretical method

2.1. Hylleraas-*B*-spine basis

The nonrelativistic Hamiltonian of helium in center-of-mass frame after eliminating system global motion is given by

$$H=\sum_i^2\left(-\frac{1}{2\mu}\nabla_i^2-\frac{2}{r_i}\right)+\frac{1}{M_{\rm N}}\nabla_1\cdot\nabla_2+\frac{1}{r_{12}},\tag{1}$$

where r_1, r_2, r_{12} denote radial distances of two electrons relative to nucleus and distance between the two electrons. $M_{\rm N}$ and μ represent the nucleus mass and reduced mass of electrons, which is in the form of $M_{\rm N}/(1+M_{\rm N})$. The nucleus mass is considered to be infinite in this article.

For a given total angular quantum number L and total magnetic quantum number M, the trial wave function could be expanded as

$$\Psi=\sum_{i,j,c}\sum_{l_1,l_2}C^{i,j,c}_{l_1,l_2}(1\pm\hat{P}_{12})B_{i,\nu}(r_1)B_{j,\nu}(r_2)r_{12}^c\mathit{\Lambda}^{LM}_{l_1l_2}(\hat{\boldsymbol{r}}_1,\hat{\boldsymbol{r}}_2).\tag{2}$$

Here $\hat{P}_{12}$ indicates the permutation between two electrons and $\pm$ is determined by total spin of basis state, $+$ for singlet states and $-$ for triplet states, respectively. $C^{i,j,c}_{l_1,l_2}$ are the linear expansion coefficients of basis functions. $B_{i,\nu}$ is the i-th ν order B-spline function. r_{12}^c is the Hylleraas factor. $\mathit{\Lambda}^{LM}_{l_1l_2}(\hat{\boldsymbol{r}}_1,\hat{\boldsymbol{r}}_2)$ is the vector coupled product of angular momenta l_1, l_2 for two electrons,

$$\mathit{\Lambda}^{LM}_{l_1l_2}(\hat{\boldsymbol{r}}_1,\hat{\boldsymbol{r}}_2)=\sum_{m_1,m_2}\langle l_1l_2m_1m_2|LM\rangle Y_{l_1}^{m_1}(\hat{\boldsymbol{r}}_1)Y_{l_2}^{m_2}(\hat{\boldsymbol{r}}_2),\tag{3}$$

where $\langle l_1l_2m_1m_2|LM\rangle$ are the Clebsch–Gordan coefficients and $\hat{\boldsymbol{r}}_i=\boldsymbol{r}_i/r_i$ $(i=1,2)$.

The overlap matrix elements O_{IJ} can be directly evaluated by

$$O_{IJ}=\sum_{qk}C_{cqk}G_1I_R(i,j,i',j',c),\tag{4}$$

where

$$C_{cqk}=\frac{2q+1}{c+2}\binom{c+2}{2k+1}\prod_{t=0}^{S_{qc}}\frac{2k+2t-c}{2k+2q-2t+1}.\tag{5}$$

Here q and k are summation indexes which rank from zero to $c/2$ and zero to $c/2-q$ for even c or from zero to infinity and zero to $(c+1)/2$ for odd c; t is continued product index, $S_{qc}=\min(q-1,(c+1)/2)$ is the upper limit value of continued product, and G_1 represents angular integral parts which are reduced from the summation of Wigner $3j$ symbol,

$$\begin{aligned}G_1\;=\;&(-1)^{L+l_2-l_2'}\delta_{LL'}\delta_{MM'}(l_1,l_1',l_2,l_2')\begin{pmatrix}l_1&q&l_1'\\0&0&0\end{pmatrix}\\&\begin{pmatrix}l_2&l_2'&q\\0&0&0\end{pmatrix}\begin{Bmatrix}L&l_1&l_2\\q&l_1'&l_2'\end{Bmatrix},\end{aligned}\tag{6}$$

where (l_1,l_1',l_2,l_2') are brief denotations of $(2l_1+1)(2l_1'+1)(2l_2+1)(2l_2'+1)$. The radial integral parts

$$\begin{aligned}&I_R(i,j,i',j',c)\\=\;&\int_0^\infty{\rm d}r_1\int_0^{r_1}{\rm d}r_2B_{i,\nu}(r_1)B_{j,\nu}(r_2)B_{i',\nu}(r_1)\\&\times B_{j',\nu}(r_2)\frac{r_1^{q+2k+2}}{r_2^{q+2k-c-2}}\\&+\int_0^\infty{\rm d}r_2\int_0^{r_2}{\rm d}r_1B_{i,\nu}(r_1)B_{j,\nu}(r_2)B_{i',\nu}(r_1)\\&\times B_{j',\nu}(r_2)\frac{r_2^{q+2k+2}}{r_1^{q+2k-c-2}}\end{aligned}\tag{7}$$

could be efficiently calculated by the Gauss–Legendre quadrature. The evaluation of matrix elements of Hamiltonian H_{IJ} involves operators of T and V. T consists of $\partial^2/\partial r_i^2$, $\partial/\partial r_i$, and $\hat{\boldsymbol{r}}_i\cdot\hat{\boldsymbol{\nabla}}_j^Y$, where $\hat{\boldsymbol{\nabla}}_j^Y=\boldsymbol{e}_{\theta_j}\partial/\partial\theta_j+\boldsymbol{e}_{\phi_j}1/\sin\theta_j\cdot\partial/\partial\phi_j$, and V could be reduced to O_{IJ}. Noticing the similarity between forms of $\partial_rB_{i,\nu}$,

$$\begin{aligned}\frac{\partial}{\partial r_i}B_{i,\nu}(r)\;=\;&\frac{\nu-1}{t_{i+\nu-1}-t_i}B_{i,\nu-1}(r)\\&-\frac{\nu-1}{t_{i+\nu}-t_{i+1}}B_{i+1,\nu-1}(r),\end{aligned}\tag{8}$$

and of the recurrence relation of $B_{i,\nu}$,

$$B_{i,\nu}(r)=\frac{r-t_i}{t_{i+\nu-1}-t_i}B_{i,\nu-1}(r)+\frac{t_{i+\nu}-r}{t_{i+\nu}-t_{i+1}}B_{i+1,\nu-1}(r),\tag{9}$$

where t_i, t_{i+1}, $t_{i+\nu-1}$, $t_{i+\nu}$ represent knots of B-spline functions, all radial part integrals of T, V and O_{IJ} could be calculated in a unified form, linear combination of integrals to $B_{i,\nu-1}(r)$'s, which reduces lots of computation. The angular integral part of $\hat{\boldsymbol{r}}_i\cdot\hat{\nabla}_j^Y$ could be calculated in the following form:

$$\begin{aligned}G_2\;=\;&\delta_{LL'}\delta_{MM'}(l_1,l_1',l_2,l_2')^{\frac{1}{2}}\sum_{T_1,T_2}b(l_2;T_2)(T_1,T_2)\\&\begin{pmatrix}1&l_1&T_1\\0&0&0\end{pmatrix}\begin{pmatrix}1&l_2&T_2\\0&0&0\end{pmatrix}\\&\begin{pmatrix}l_1'&T_1&q\\0&0&0\end{pmatrix}\begin{pmatrix}l_2'&T_2&q\\0&0&0\end{pmatrix}\\&\begin{Bmatrix}T_2&l_2&1\\l_1&T_1&L\end{Bmatrix}\begin{Bmatrix}l_2'&T_2&q\\T_1&l_1'&L\end{Bmatrix}.\end{aligned}\tag{10}$$

Here b is equal to l_2+1 when $T_1 = l_2-1$, or equal to $-l_2$ when $T_2 = l_2+1$, T_1 and T_2 are summation indexes, and (T_1, T_2) is brief denotation of $(2T_1+1)(2T_2+1)$.

2.2. Geometric quantities

The evaluation of quantities $\langle r\rangle$, $\langle r_{12}\rangle$, $\langle r_<\rangle$, $\langle r_>\rangle$, $\langle\cos\theta_{12}\rangle$ and $\langle\theta_{12}\rangle$ could be dealt by including corresponding term into O_{IJ}. For angular quantities $\langle\theta_{12}\rangle$, the multipole expansion method is adopted to investigate its expectation values

$$\langle\theta_{12}\rangle = \frac{1}{2}\sum_{k=0}^{\infty}(2k+1)I_{1,k}q_k, \tag{11}$$

where

$$q_k = \langle P_k(\cos\theta_{12})\rangle \tag{12}$$

and

$$\begin{aligned} I_{1,k} &= \int_0^{\pi} \mathrm{d}\theta_{12}\sin\theta_{12}P_k(\cos\theta_{12})\theta_{12} \\ &= \int_{-1}^{1}\mathrm{d}xP_k(x)\arccos(x). \end{aligned} \tag{13}$$

The expansion coefficient $I_{1,k}$ could be performed analytically.[24] $I_{1,k}$ is equal to $\pi\delta_{k/2,0}$ when k is even, or is equal to

$$\pi\sum_{i=0}^{m}(-1)^{m-i}\frac{(2m+2i+1)!!}{(2i+2)!(2m-2i)!!}\left[\frac{(2i+1)!!}{(2i+2)!!}-1\right], \tag{14}$$

where $m = (k-1)/2$ when k is odd. The calculation of $q_k = \langle P_k(\cos\theta_{12})\rangle$ could be dealt with the help of

$$P_k(\cos\theta_{12}) = \frac{4\pi}{2k+1}\sum_{q=-k}^{k}Y_k^q(\hat{r}_1)^*Y_k^q(\hat{r}_2). \tag{15}$$

This angular integral part is similar to Eq. (10), which just needs to adjust the number 1 to k in all Wigner $3j$ and $6j$ symbols.

3. Results and discussions

3.1. Energy levels

Table 1 shows a convergence study of energy level for doubly excited $2p^2\,{}^3P^e$ state of helium with increasing total number of B-spline N and partial-wave expansion length l_{max}. As shown in this table, the results of this state converge to $E = -0.710\,500\,155\,6$ when $l_{max} = 4$. The extrapolated energy level of this state is $E = -0.710\,500\,155\,67(1)$, which has 11 significant digits and are consistent with precise values $E = -0.710\,500\,155\,678\,3$ and $E = -0.710\,500\,155\,678\,33$ obtained from the exponential correlated basis[25] and the extensive Hylleraas-CI method.[4]

Table 1. Convergence study of the energy level for the $2p^2\,{}^3P^e$ state of helium as the total number of B-splines N and the partial-wave expansion length l_{max} increase. The numbers in parentheses of the extrapolated values are the computational uncertainties. Here all the data are in units of a.u.

$N\backslash l_{max}$	2	3	4
30	–0.710 500 11	–0.710 500 13	–0.710 500 14
35	–0.710 500 150	–0.710 500 153 1	–0.710 500 154
40	–0.710 500 154 3	–0.710 500 155 2	–0.710 500 155 4
45	–0.710 500 154 82	–0.710 500 155 60	–0.710 500 155 62
50	–0.710 500 154 89	–0.710 500 155 659	–0.710 500 155 665
∞			–0.710 500 155 67(1)

Table 2 displays our extrapolated energy levels for $2pnp\,{}^1P^e$ $(3 \le n \le 5)$ and $2pnp\,{}^3P^e$ $(2 \le n \le 5)$ states. Comparisons with other precise results are available. Reference data a come from the results of Eiglsperger *et al.* calculated with Coulomb–Sturmian basis CI method.[9] Reference data b represent results from Kar and Ho using exponential correlated wave functions.[25] Reference data c are obtained by Hilger using extensive Hylleraas-CI calculation.[4] Our results are more consistent with reference data c which are the most accurate known results for these nonautoionization states. Compared to reference data a, Our results have 2 significant digits more precise for $2pnp\,{}^1P^e$ with $n = 3, 4$, and 4 significant digits for $2p4p\,{}^3P^e$ states.

Table 2. Extrapolated energy levels of doubly excited bound $2pnp\,{}^1P^e$ $(3 \le n \le 5)$ and $2pnp\,{}^3P^e$ $(2 \le n \le 5)$ states of helium in comparison with reference data. The numbers in parentheses of the extrapolated values are the computational uncertainties. Here all the data are in units of a.u.

	$^1P^e$		$^3P^e$	
n	Present work	Reference data	Present work	Reference data
2			–0.710 500 155 67(1)	–0.710 499 8[a]
				–0.710 500 155 678 3[b]
				–0.710 500 155 678 33[c]
3	–0.580 246 472 6(1)	–0.580 246 471 5[a]	–0.567 812 898 72(1)	-0.567 812 81[a]
		–0.580 246 472 594[b]		–0.567 812 898 724[b]
		–0.580 246 472 594 38[c]		–0.567 812 898 725 152[c]
4	–0.540 041 590 936(3)	–0.540 041 590 5[a]	–0.535 867 188 766(3)	–0.535 867 15[a]
		–0.540 041 590 09[b]		–0.535 867 188 7[b]
		–0.540 041 590 938 51[c]		–0.535 867 188 768 21[c]
5	–0.524 178 981 809(3)	–0.524 178 981 6[a]	–0.522 254 575 705(3)	–0.522 254 56[a]
		–0.524 179 0[b]		–0.522 254 57[b]
		–0.524 178 981 811 41[c]		–0.522 254 575 707 23[c]

[a]Ref. [9], [b]Ref. [25], [c]Ref. [4].

Table 3 displays a comparison of energy levels for $2pnd\,^{1,3}D^{o}\,(3 \le n \le 5)$ states. In this table, reference data d come from results of Bhattacharyya calculated with an extended Hylleraas basis.[26] For these $2pnd\,^{1,3}D^{o}\,(3 \le n \le 5)$ states, our results are more consistent with reference data b, the most precise known results of these energy levels. Our results have at least 2 significant digits more accurate than reference data a and d for all $2pnd\,^{1,3}D^{o}\,(3 \le n \le 5)$ states. These results indicate that for higher doubly excited bound states, precise energy levels could be acquired using the H-*B*-spline basis without too large increase of total number of *B*-spline *N*. As we can see, the energy levels for higher excited states, either for $^{1,3}P^{e}$ or $^{1,3}D^{o}$ states, have more convergency significant digits than lower excited states, mainly due to the knots of *B*-spline functions we choose to make the H-*B*-spline basis more appropriate to fit wavefunctions of higher excited states, which distribute in a broader radial range, and the interelectronic correlated effect is weak. The results also provide the precise wavefunctions for the following calculations.

Table 3. Extrapolated energy levels of doubly excited bound $2pnd\,^{1,3}D^{e}\,(3 \le n \le 5)$ states of helium in comparison with reference data. The numbers in parentheses of the extrapolated values are the computational uncertainties. Here all the data are in units of a.u.

	$^1D^o$		$^3D^o$	
n	Present work	Reference data	Present work	Reference data
3	–0.563 800 420 46(1)	–0.563 800 418[a]	–0.559 328 263 09(1)	–0.559 328 24[a]
		–0.563 800 420 462[b]		–0.559 328 263 096[b]
		–0.563 800 42[d]		–0.559 328 26[d]
4	–0.534 576 385 554(1)	–0.534 576 384 8[a]	–0.532 678 601 89(1)	–0.532 678 59[a]
		–0.534 576 385 556[b]		–0.532 678 601 895[b]
		–0.534 576 38[d]		–0.532 678 60[d]
5	–0.521 659 015 464(4)	–0.521 659 015 1[a]	–0.520 703 462 026(4)	–0.520 703 455[a]
		–0.521 659 015 466[b]		–0.520 703 462 028[b]
		–0.521 659 01[d]		–0.520 703 45[d]

[a]Ref. [9], [b]Ref. [25], [c]Ref. [26].

3.2. Geometric quantities

The H-*B*-spline basis has shown its well capacity in calculation on energy levels for lower lying doubly excited bound states of helium. Here we use this basis to calculate the expectation values of geometric quantities $\langle r\rangle$, $\langle r_{12}\rangle$, $\langle r_<\rangle$, $\langle r_>\rangle$, $\langle\cos\theta_{12}\rangle$ and $\langle\theta_{12}\rangle$ in detail. As mentioned in Section 2, the investigation on $\langle\theta_{12}\rangle$ is carried out by multipole expansion. Table 4 presents the contributions of the first 17 order expansion terms to the expectation value $\langle\theta_{12}\rangle$ for $2p^2\,^3P^e$ state under total number of *B*-spline $N = 50$ and partial-wave expansion length $l_{max} = 4$. As displayed in this table, the contribution of $\langle P_k(\cos\theta_{12})\rangle$ reaches the magnitude of 10^{-9} at $k = 17$, and the changes of values of $\langle\theta_{12}\rangle$ are quite small. We truncate the summation (11) to $k_{max} = 17$ in our calculations and extrapolate these values to give the computational uncertainties.

Expectation values of all geometric quantities are carried out under $l_{max} = 4$ in the following calculations. Table 5 displays extrapolated expectation values of radial quantities $\langle r_<\rangle, \langle r_>\rangle, \langle r\rangle$ and $\langle r_{12}\rangle$ for $2pnp\,^1P^e\,(3 \le n \le 5)$, $2pnp\,^3P^e\,(2 \le n \le 5)$ and $2pnd\,^{1,3}D^o\,(3 \le n \le 5)$ states. All expectation values of radial quantities listed in Table 5 have at least 10 significant digits and these results satisfy the relation $2\langle r\rangle = \langle r_<\rangle + \langle r_>\rangle$ within the absolute difference of 10^{-9}. Table 6 displays extrapolated expectation values of angular quantities $\langle\cos\theta_{12}\rangle$ and $\langle\theta_{12}\rangle$ for these states. Extrapolated expectation values of $\langle\cos\theta_{12}\rangle$ have at least 10 significant digits and $\langle\theta_{12}\rangle$ at least 7 significant digits. The results presented in Table 6 satisfy the second order approximate formula of interelectronic angular expectation value $\langle\theta_{12}\rangle$, $\langle\theta_{12}\rangle \approx \frac{\pi}{2} + \frac{3\pi}{8}\langle\cos\theta_{12}\rangle$. The results converge to the Rydberg limits 90° as principle quantum number *n* increases. To our best knowledge, there are less precise results available for these states. Our results could provide benchmark values for future related studies.

Table 4. Contributions of the first 17 order expansion terms to the interelectronic angle expectation value $\langle\theta_{12}\rangle$ for doubly excited bound $2p^2\,^3P^e$ state of helium. Here all the data are in units of a.u.

k	q_k	$I_{1,k}$	$(2k+1)q_kI_{1,k}$	$\langle\theta_{12}\rangle$
1	$-7.140371751620546\times10^{-2}$	-2.50000×10^{-1}	$5.355278813715409\times10^{-2}$	94.819750932
3	$2.961440797912420\times10^{-2}$	-1.56250×10^{-2}	$-3.239075872716709\times10^{-3}$	94.528234103
5	$4.970328659624325\times10^{-4}$	-3.90625×10^{-3}	$-2.135688095932327\times10^{-5}$	94.526311984
7	$6.419211633705366\times10^{-5}$	-1.52588×10^{-3}	$-1.469240943993842\times10^{-6}$	94.526179752
9	$1.454986959503822\times10^{-5}$	-7.47681×10^{-4}	$-2.066944670559781\times10^{-7}$	94.526161150
11	$4.474630535892804\times10^{-6}$	-4.20570×10^{-4}	$-4.328363182598181\times10^{-8}$	94.526157254
13	$1.677933193840126\times10^{-6}$	-2.59638×10^{-4}	$-1.176268331968336\times10^{-8}$	94.526156196
15	$7.209572193986499\times10^{-7}$	-1.71402×10^{-4}	$-3.830768462341050\times10^{-9}$	94.526155851
17	$3.154052627862183\times10^{-7}$	-1.19029×10^{-4}	$-1.313981353625644\times10^{-9}$	94.526155733

Table 5. Expectation values of radial geometric quantities for doubly excited bound $2pnp\,^1P^e\,(3 \le n \le 5)$, $2pnp\,^3P^e\,(2 \le n \le 5)$ and $2pnd\,^{1,3}D^o\,(3 \le n \le 5)$ states of helium. The numbers in parentheses of the extrapolated values are the computational uncertainties. Here all the data are in units of a.u.

State	$\langle r_< \rangle$	$\langle r_> \rangle$	$\langle r \rangle$	$\langle r_{12} \rangle$
$2p3p\,^1P^e$	2.403 694 703(1)	8.971 272 732(2)	5.687 483 717(1)	9.383 100 169(2)
$2p4p\,^1P^e$	2.469 125 391 7(2)	18.109 904 482(4)	10.289 514 93(1)	18.333 217 05(1)
$2p5p\,^1P^e$	2.485 927 618(1)	30.297 333 19(1)	16.391 630 40(1)	30.435 628 27(1)
$2p2p\,^3P^e$	2.213 050 154(1)	3.966 707 911(1)	3.089 879 033(1)	4.676 371 886(1)
$2p3p\,^3P^e$	2.509 554 589(1)	10.410 759 457(5)	6.460 157 023(1)	10.831 719 973(2)
$2p4p\,^3P^e$	2.506 950 068 9(2)	20.107 940 56(1)	11.307 445 31(1)	20.337 434 61(1)
$2p5p\,^3P^e$	2.503 962 438(1)	32.837 781 98(1)	17.670 872 21(1)	32.980 000 7(1)
$2p3d\,^1D^o$	2.545 899 079(1)	8.742 676 639(3)	5.644 287 859(1)	9.337 543 533(3)
$2p4d\,^1D^o$	2.512 276 843 0(2)	18.724 221 38(1)	10.618 249 11(1)	19.004 925 26(1)
$2p5d\,^1D^o$	2.504 993 527 7(3)	31.665 481 72(1)	17.085 237 62(1)	31.829 444 93(1)
$2p3d\,^3D^o$	2.510 005 646(1)	9.767 375 714(3)	6.138 690 680(1)	10.164 456 60(1)
$2p4d\,^3D^o$	2.502 332 979(1)	20.029 042 64(1)	11.265 687 813(2)	20.240 904 64(1)
$2p5d\,^3D^o$	2.500 905 931 3(3)	33.280 537 6(1)	17.890 721 80(1)	33.412 743 3(1)

Table 6. Expectation values of angular geometric quantities for doubly excited bound $2pnp\,^1P^e\,(3 \le n \le 5)$, $2pnp\,^3P^e\,(2 \le n \le 5)$ and $2pnd\,^{1,3}D^o\,(3 \le n \le 5)$ states of helium. The numbers in parentheses of the extrapolated values are the computational uncertainties. Here all the data are in units of a.u.

State	$\langle \cos\theta_{12} \rangle$	$\langle \theta_{12} \rangle$	State	$\langle \cos\theta_{12} \rangle$	$\langle \theta_{12} \rangle$
$2p3p\,^1P^e$	$-3.198\,513\,530(1)\times10^{-2}$	92.026 152(1)	$2p3d\,^1D^e$	$-6.833\,318\,740\,6(2)\times10^{-2}$	94.324 538(1)
$2p4p\,^1P^e$	$-1.274\,515\,627\,5(4)\times10^{-2}$	90.807 139(1)	$2p4d\,^1D^e$	$-2.533\,389\,665\,6(1)\times10^{-2}$	91.603 143 5(1)
$2p5p\,^1P^e$	$-6.212\,482\,975(3)\times10^{-3}$	90.393 391(1)	$2p5d\,^1D^e$	$-1.211\,799\,286\,3(2)\times10^{-2}$	90.766 814 0(1)
$2p2p\,^3P^e$	$-7.140\,371\,751\,0(6)\times10^{-2}$	94.526 155(1)			
$2p3p\,^3P^e$	$-3.122\,960\,724\,0(3)\times10^{-2}$	91.978 39(1)	$2p3d\,^3D^e$	$-1.605\,510\,687\,1(1)\times10^{-2}$	91.020 058(2)
$2p4p\,^3P^e$	$-1.339\,606\,321\,2(2)\times10^{-2}$	90.848 459(1)	$2p4d\,^3D^e$	$-6.109\,212\,513\,3(6)\times10^{-3}$	90.388 113(1)
$2p5p\,^3P^e$	$-6.806\,335\,012(2)\times10^{-3}$	90.431 052 2(1)	$2p5d\,^3D^e$	$-3.037\,907\,948(1)\times10^{-3}$	90.192 974(3)

4. Summary

In this article, the Hylleraas-*B*-spline basis is imported into the calculation of energy levels for doubly excited $2pnp\,^1P^e\,(3 \le n \le 5)$, $2pnp\,^3P^e\,(2 \le n \le 5)$ and $2pnd\,^{1,3}D^o\,(3 \le n \le 5)$ states of helium. Good agreement is achieved between our results and the precise values obtained by Kar and Ho[25] and Hilger *et al.*[4] Geometric quantities $\langle r_< \rangle$, $\langle r_> \rangle$, $\langle r \rangle$, $\langle r_{12} \rangle$, $\langle \cos\theta_{12} \rangle$ and $\langle \theta_{12} \rangle$ of these states are investigated in detail as well and precise results are reported. Our results of these geometric quantities provide a precise reference for future studies.These calculations have shown the good capacity of the H-*B*-spline basis in calculation on lower lying doubly excited bound states. It would be appealing to an extend H-*B*-spline basis to the calculations of doubly excited resonance states of helium accompanied with stabilization and complex-rotation method.

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