

## Comment on “Doubly excited bound and resonance ( ${}^3P^e$ ) states of helium”

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Recently a study [J. K. Saha and T. K. Mukherjee, *Phys. Rev. A* **80**, 022513 (2009)] on the doubly excited  ${}^3P^e$  states of helium reports some resonance states that are not in conformity with previously published works [Y. K. Ho and A. K. Bhatia, *Phys. Rev. A* **47**, 2628 (1993)]. Owing to discrepancies between the works, we investigate the resonance parameters (positions and widths) of the doubly excited Feshbach resonances of the  ${}^3P^e$  symmetries associated with  $N = 3, 4$ , and  $5 \text{ He}^+$  thresholds using a different choice of correlated wave functions in the framework of the complex-coordinate rotation method and the stabilization method. Resonance parameters below the  $N = 4$  and  $N = 5 \text{ He}^+$  thresholds obtained from the present calculations are not consistent with the results and discussions made in the recent work. Here we point out an error in assessment made by Saha and Mukherjee in an earlier work as well as the lack of numerical accuracy of the results for some high-lying doubly excited states reported by Saha and Mukherjee. The bound  $2p^2 {}^3P^e$  and  $2p3p {}^3P^e$  state energies obtained from this calculation are consistent with the best reported results but not with the reported values of Saha and Mukherjee.

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Investigation of doubly excited states of helium atoms using highly correlated wave functions is of special interest because these states can be determined precisely. Results with a high degree of accuracy can be achieved depending on the accuracy of the wave functions and computational performance. Recently, a study [1] on the doubly excited  ${}^3P^e$  states of helium using the stabilization method reports some resonance states that are not in conformity with previously published works [2] using the complex-coordinate rotation (CCR) method. This study [1] also reported metastable bound state energies much lower than the best reported results [3]. The main purpose of this Comment is to clarify the discrepancies of the results reported in recent works [1]. In the present work, we employ a different type of correlated wave function than used in the previous works [1,2]. We have also reoptimized our calculation on the  $2p^2 {}^3P^e$  and  $2p3p {}^3P^e$  state energies of the helium atom with an increasing number of basis terms [4,5]. Several theoretical works have been reported on the metastable bound  $2p^2 {}^3P^e$  states of helium [6–15]. The  ${}^3P^e$  resonance energies of He below the  $N = 3 \text{ He}^+$  threshold have also been reported [15]. Besides such theoretical developments, several experiments have also been performed on the doubly excited  ${}^3P^e$  state ([16,17], and references therein).

To extract resonance parameters, we have used the CCR [18–20] and stabilization methods [21–27]. Highly accurate correlated exponential wave functions with exponents generated by a quasirandom process are used to represent the correlation effect. In the present work, we have identified two, three, and four series of resonances below the  $N = 3, 4$ , and  $5 \text{ He}^+$  thresholds, respectively. All calculations are performed in quadruple precision arithmetic (32 significant figures) on IBM and ALPHA-DEC work stations in the UNIX, FEDORA, and CENT operating systems. Atomic units (a.u.) are used throughout this work. We have examined the convergence of the calculations with the increasing number of terms in the basis functions. Owing to experimental interest in  ${}^3P^e$  states,

and to the discrepancy of a recent work [1] with previously published work [2], it is important to reinvestigate the doubly excited  ${}^3P^e$  states using a different type of correlated wave function. Details on the doubly excited nonautoionizing and autoionizing states can be found in earlier works [1–15].

The nonrelativistic Hamiltonian describing the helium atom is

$$H = T + V = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - 2\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{1}{r_{12}}, \quad (1)$$

where  $r_1$  and  $r_2$  are the radial coordinates of the two electrons, and  $r_{12}$  is their relative distance. For triplet  $P$  unnatural parity states of the He atom, we employ highly correlated wave functions [27–29]:

$$\Psi = (1 - \hat{P}_{12}) \sum_{i=1}^{N_b} \sum_{l_1=\varepsilon}^L A_i (-1)^\varepsilon Y_{LM}^{l_1, l_2}(\mathbf{r}_1, \mathbf{r}_2) \times \exp [(-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12})\omega], \quad (2)$$

with

$$\mathbf{Y}_{LM}^{l_1, l_2}(\mathbf{r}_1, \mathbf{r}_2) = r_1^{l_1} r_2^{l_2} \sum_{m_1, m_2} C_{l_1 m_1, l_2 m_2}^{LM} Y_{l_1 m_1}(\hat{r}_1) Y_{l_2 m_2}(\hat{r}_2), \quad (3)$$

where the functions  $\mathbf{Y}_{LM}^{l_1, l_2}(\mathbf{r}_1, \mathbf{r}_2)$  are the bipolar harmonics or Schwartz harmonics,  $\hat{r}_i = \mathbf{r}_i / r_i$  ( $i = 1, 2$ );  $Y_{l_i m_i}(\hat{r}_i)$  denotes the usual spherical harmonics;  $C_{l_1 m_1, l_2 m_2}^{LM}$  are the Clebsch-Gordan coefficients;  $\alpha_i, \beta_i, \gamma_i$  are the nonlinear variation parameters;  $A_i$  ( $i = 1, \dots, N$ ) are the linear expansion coefficients;  $l_1 + l_2 = L + \varepsilon$ ,  $L = 1, \varepsilon = 1, N_b$  is the number of basis terms; and the operator  $\hat{P}_{12}$  is the permutation of the two identical particles 1 and 2. The scaling factor  $\omega$  is set equal to 1 for bound state calculations and is varied for resonance state calculations. Following a quasirandom process [4,5,27], the nonlinear parameters  $\alpha_i, \beta_i$ , and  $\gamma_i$  are chosen from the three

TABLE I. Doubly excited  $^3P^e$  resonance states of helium below the  $N = 4$  and  $N = 5$   $\text{He}^+$  thresholds. The numbers in the square brackets denote the powers of 10. The numbers in the subscripts show the uncertainty in the last digit.

State	Present work, complex-rotation method (using exponential wave functions)		Saha and Mukherjee [1], stabilization method (using Hylleraas-type wave functions)		Ho and Bhatia [2], complex-rotation method (using Hylleraas-type wave functions)	
	$E_r$	$\Gamma/2$	$E_r$	$\Gamma/2$	$E_r$	$\Gamma/2$
$E_{\text{th}}(N = 4) = -0.125$						
4p4p	-0.194 442 1 <sub>1</sub>	0.165 283 <sub>2</sub> [-2]	-0.197 38	0.163 5[-2]	-0.194 442	0.165 25[-2]
4d4d	-0.178 256 9 <sub>1</sub>	0.240 322 <sub>1</sub> [-2]	-0.178 78	0.229 5[-2]	-0.178 257	0.240 35[-2]
4p5p	-0.161 223 0 <sub>1</sub>	0.951 5 <sub>1</sub> [-3]	-0.161 36	0.945[-3]	-0.161 223	0.951[-3]
4f4f	-0.155 176 8 <sub>1</sub>	0.129 251 <sub>2</sub> [-3]	-0.155 20	0.135[-3]	-0.155 176 8	0.129 25[-3]
4d5d	-0.151 549 8 <sub>1</sub>	0.883 2 <sub>1</sub> [-3]	-0.151 54	0.77[-3]	-0.151 549 5	0.883[-3]
4p6p	-0.148 032 2 <sub>2</sub>	0.525 0 <sub>2</sub> [-3]	-0.148 08	0.84[-3]	-0.148 031 5	0.525[-3]
4f5f	-0.142 341 4 <sub>2</sub>	0.164 2 <sub>2</sub> [-3]	-0.142 35	0.255[-3]	-0.142 341 5	0.164 25[-3]
4d6d	-0.142 341 1 <sub>2</sub>	0.419 2 <sub>4</sub> [-3]	-0.142 07	0.370[-3]	-0.142 341	0.418 95[-3]
4p7p	-0.140 841 <sub>1</sub>	0.288 1 <sub>1</sub> [-3]	-0.140 90	0.400[-3]	-0.140 84	0.285[-3]
4d7d	-0.137 293 <sub>1</sub>	0.311 <sub>2</sub> [-3]	-0.137 42	0.290[-3]	-0.137 295	0.306[-3]
4f6f	-0.137 152 <sub>2</sub>	0.562 <sub>4</sub> [-4]	-0.137 16	0.55[-4]	-0.137 15	0.55[-4]
4p8p	-0.136 52 <sub>1</sub>	0.164 <sub>3</sub> [-3]	-0.136 55	0.24[-3]		
4d8d	-0.134 180 <sub>1</sub>	0.22 <sub>1</sub> [-3]	-0.134 05	0.20[-4]		
4f7f	-0.134 07 <sub>1</sub>	0.32 <sub>3</sub> [-4]	-0.133 75	0.90[-4]		
$E_{\text{th}}(N = 5) = -0.08$						
5p5p	-0.126 378 <sub>2</sub>	0.108 7 <sub>1</sub> [-2]			-0.126 39	0.108 5[-2]
5d5d	-0.119 301 <sub>1</sub>	0.176 9 <sub>1</sub> [-2]	-0.119 37	0.875[-3]	-0.119 30	0.177[-2]
5f5f	-0.109 463 <sub>1</sub>	0.156 1 <sub>1</sub> [-2]	-0.109 96	0.925[-3]	-0.109 463	0.156 1[-2]
5p6p	-0.107 265 <sub>1</sub>	0.765 <sub>1</sub> [-3]	-0.107 65	0.5[-3]	-0.107 265	0.765[-3]
5g5g	-0.102 097 <sub>2</sub>	0.113 5 <sub>2</sub> [-3]	-0.102 99	0.102[-2]	-0.102 096	0.113 45[-3]
5d6d	-0.098 602 <sub>1</sub>	0.453 <sub>1</sub> [-3]	-0.098 28	0.424[-3]	-0.098 602	0.453[-3]
5f6f	-0.096 64 <sub>1</sub>	0.689 <sub>1</sub> [-3]	-0.096 56	0.453[-3]	-0.096 640 5	0.637[-3]
5g6g	-0.095 254 <sub>1</sub>	0.442 <sub>2</sub> [-4]	-0.095 26	0.201[-3]	-0.095 253 85	0.442 5[-4]
5p7p	-0.095 131 <sub>2</sub>	0.743 <sub>1</sub> [-3]			-0.095 13	0.74[-3]
5d7d	-0.093 44 <sub>1</sub>	0.22 <sub>1</sub> [-3]	-0.093 65	0.226 5[-3]	-0.093 44	0.205[-3]
5f7f	-0.091 51 <sub>1</sub>	0.48 <sub>2</sub> [-3]	-0.091 66	0.327[-3]	-0.091 51	0.425[-3]
5p8p	-0.091 11 <sub>2</sub>	0.43 <sub>1</sub> [-3]	-0.091 12	0.368 5[-3]	-0.091 105	0.43[-3]
5g7g	-0.090 725 <sub>1</sub>	0.21 <sub>1</sub> [-4]	-0.090 72	0.172 5[-4]	-0.090 724 5	0.21[-4]
5d8d	-0.090 245 <sub>2</sub>	0.521 <sub>1</sub> [-4]	-0.090 26	0.127[-3]		
5f8f	-0.088 63 <sub>1</sub>	0.31 <sub>2</sub> [-3]	-0.089 08	0.299 5[-3]		

positive intervals  $[A_1, A_2]$ ,  $[B_1, B_2]$ , and  $[C_1, C_2]$  and are written in matrix form as

$$\{\alpha_i \quad \beta_i \quad \gamma_i\} = \{\langle\langle k\sqrt{2}\rangle\rangle A_{21} + A_1 \quad \langle\langle k\sqrt{3}\rangle\rangle B_{21} + B_1 \quad \langle\langle k\sqrt{5}\rangle\rangle C_{21} + C_1\}, \quad (4)$$

where the symbol  $\langle\langle \dots \rangle\rangle$  denotes the fractional part of a real number,  $k = i(i + 1)/2$ ,  $A_{21} = A_2 - A_1$ ,  $B_{21} = B_2 - B_1$ ,  $C_{21} = C_2 - C_1$ . The exponential wave functions supported by the quasirandom process are widely used in several other works [4,5,27–29]. We have used the stabilization method [21–27] and the complex-rotation method to extract resonance parameters [18–20].

In the stabilization method, a resonance position can be identified from the flat plateau of the stabilization diagram, obtained by plotting the energy level  $E(\omega)$  for varying  $\omega$ . To extract resonance parameters (resonance position,  $E_r$ , and resonance width,  $\Gamma$ ) for a particular resonance state, we calculate the density of the resonance states,  $\rho_n(E)$ , in the stabilized plateau for each single energy level in the

stabilization diagram following the earlier works of Ho *et al.* [21–27]. After calculating  $\rho_n(E)$  for all the energy levels of the stabilization diagram, we fit these  $\rho_n(E)$ , one set at a time, to the Lorentzian form as used in earlier works [21–27]. The fit that gives the best fit [27] to the Lorentzian form is considered the desired result for that particular resonance. Using the stabilization method, we are able to extract the  $3pnp \ ^3P^e$  ( $n = 3-9$ ) and  $3dnd \ ^3P^e$  ( $n = 3-8$ ) resonance parameters. These resonance parameters below the  $N = 3 \ \text{He}^+$  threshold are in reasonable agreement with those reported by Saha and Mukherjee [1] and in good agreement with those reported by Ho and Bhatia [2].

In the CCR method [18–20,29], the interparticle radial coordinates  $r_{ij}$  are transformed into  $r_{ij} = r_{ij} \exp(i\theta)$ , where  $\theta$  is real and positive. The Hamiltonian  $H$  takes the form

$$H = T \exp(-2i\theta) + V \exp(-i\theta). \quad (5)$$

Under such a transformation, one needs to calculate the matrix element for the kinetic energy term and the potential energy

TABLE II. Effective quantum numbers  $n^*$  and effective resonance widths  $(n^*)^3\Gamma$  for the  ${}^3P^e$  states of He below the  $N = 4$  and  $N = 5$  He $^+$  thresholds,  $E_{th}$ .

$E_{th}(N = 4) = -0.125$ a.u.			$E_{th}(N = 5) = -0.08$		
State	$n^*$	$(n^*)^3\Gamma$	State	$n^*$	$(n^*)^3\Gamma$
4p4p	2.683 326 9	0.063 867 4	5p5p	3.283 439 2	0.076 956 7
4d4d	3.064 058 6	0.138 265 8	5d5d	3.566 836 5	0.160 548 9
4p5p	3.715 290 6	0.097 592 7	5f5f	4.119 519 1	0.218 259 2
4f4f	4.070 505 4	0.017 434 5	5p6p	4.282 350 9	0.120 154 0
4d5d	4.339 646 7	0.144 361 8	5g5g	4.756 837 8	0.024 433 2
4p6p	4.659 263 7	0.106 204 1	5d6d	5.184 479 7	0.126 253 6
4f5f	5.369 612 2	0.050 843 1	5f6f	5.481 612 6	0.226 973 0
4d6d	5.369 658 7	0.129 805 0	5g6g	5.725 232 5	0.016 589 4
4p7p	5.618 154 8	0.102 177 3	5p7p	5.748 455 7	0.282 275 0
4d7d	6.377 582 1	0.161 346 1	5d7d	6.099 375 5	0.099 841 0
4f6f	6.414 475 1	0.029 665 4	5f7f	6.590 939 7	0.274 861 1
4p8p	6.588 078 5	0.093 788 6	5p8p	6.708 539 4	0.259 646 4
4d8d	7.380 124 0	0.176 865 7	5g7g	6.827 887 4	0.0133 693
4f7f	7.424 741 9	0.026 195 3	5d8d	6.986 007 1	0.035 526 7
			5f8f	7.611 663 9	0.273 420 1

term of Eq. (1) separately and then scale them according to Eq. (5). Resonance position can be identified by observing the complex energy levels  $E(\theta, \omega)$ . The resonance positions and widths can be extracted when the discrete complex eigenvalues are stabilized with respect to the nonlinear parameters in the wave functions and to the rotational angle  $\theta$ . The complex resonance eigenvalue  $W = E_r - i\Gamma/2$  corresponding to the stationary region represents the resonance energy,  $E_r$ , and the width,  $\Gamma$ . For the details of the complex-rotation method, readers are referred to review articles [18]. Using the CCR method, we have extracted resonance parameters below the  $N = 3, 4$ , and  $5$  thresholds of He $^+$ . Resonance parameters below the  $N = 4$  and  $N = 5$  He $^+$  thresholds are presented in Table I. The number  $x$  in the superscript in Table I shows the uncertainty in the resonance parameters in the last quoted digits that would be lying in the range  $(-x, x)$ .

To classify the resonance states below the  $N = 4$  and  $N = 5$  thresholds, we have calculated the effective widths,  $(n^*)^3\Gamma$ . The effective quantum number  $(n^*)$  for  ${}^3P^e$  resonance states are obtained using the formula

$$E = -\frac{1}{2} \left[ \left( \frac{Z}{N} \right)^2 + \left( \frac{Z-1}{n^*} \right)^2 \right], \quad (6)$$

TABLE III. Comparisons of the bound-excited metastable  ${}^3P^e$  state energies with the other calculations.

Calculation	$E(2p^2\,{}^3P^e)$ (a.u.)	$E(2p3p\,{}^3P^e)$ (a.u.)
Using 700-term basis functions (2)	-0.710 500 155 678 316	-0.567 812 898 724 643
Using 800-term basis functions (2)	-0.710 500 155 678 338	-0.567 812 898 725 080
Using 900-term basis functions (2)	-0.710 500 155 678 339	-0.567 812 898 725 396
Other calculations		
Saha <i>et al.</i> [1]	-0.710 500 165 215 26	-0.567 812 899 807 06
Hilger <i>et al.</i> [3]	-0.710 500 155 678 33	-0.567 812 898 725 15
Kar and Ho [4]	-0.710 500 155 678 3	
Mukherjee <i>et al.</i> [12]	-0.710 500 155 656 78	

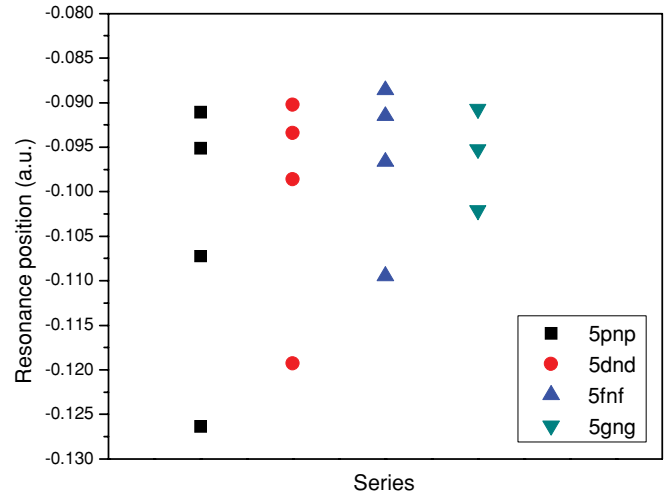


FIG. 1. (Color online) Energy level diagram for different series of resonance states associated with, and converging on, the  $N = 5$  He $^+$  threshold (threshold energy  $-0.080$  a.u.), with  $n \geq 5$ .

where  $N, E$ , and  $Z$  denote the inner electron quantum number, the energy of the state below the total ionization, and the atomic number, respectively. We present the effective quantum numbers and the effective resonance widths in Table II. Our calculated resonance parameters are in good accordance with the reported results of Ho and Bhatia [2]. Ho and Bhatia have employed correlated Hylleraas-type wave functions involving the powers of interparticle distances. Our work is comparable with the reported resonance parameters of Saha and Mukherjee [1] below the  $N = 3$  threshold (not shown here because of limited page space). However, the result is not in agreement below the  $N = 4$  and  $N = 5$  thresholds. As in the work of Ho and Bhatia [2], we have obtained the seventh and eighth  ${}^3P^e$  resonance positions  $E_r$  below the  $N = 4$  threshold at  $-0.142\,341\,4$  a.u. and  $-0.142\,341$  a.u., respectively, and these are the members of two different series (see Table II) having different widths. These two resonance states are not in agreement with the reported resonance parameters of Saha and Mukherjee [1]. It appears from Table I that their calculated results lose accuracy from this state to all the higher lying states. We have also obtained the resonance energy of  $-0.095\,13$  a.u. for the eighth resonance state below the  $N = 5$  threshold, which are in conformity with Ho and Bhatia [2] but not in agreement with Saha and Mukherjee [1]. It is also important to mention here that the stabilization method can

produce resonance parameters for some lower lying states depending on the size of the basis; however, accurate resonance position and resonance widths can be obtained using the CCR method. The spacing statement in the energy level diagram (see Fig. 4 of [1]) presented in Ref. [1] is not valid for resonance states with multiple series converging on a given excited state of the  $\text{He}^+$  threshold but is valid for bound states or bound metastable states with only one series. For the resonances associated with the  $\text{He}^+$  ( $N = 5$ ) threshold, Saha and Mukherjee [1] did not find agreement with those resonances in Ref. [2] and concluded that one of the  $N = 5$  states reported in Ref. [2] should be discarded. But this was an error in assessment made by Saha and Mukherjee [1]. The correct interpretation of the present results and of those in Ref. [2] is the following. For doubly excited  $5nl' \ ^3P^e$  states, there are four series converging on the  $N = 5$   $\text{He}^+$  threshold. They are the  $5pnp$ ,  $5dnd$ ,  $5fnf$ , and  $5ngg$  states, with  $n \geq 5$  series. We present the energy levels for the different series of resonance states in Fig. 1. The degeneracy in the resonance energy having different resonance widths confirms their existence in different series. The large difference in the resonance widths below the  $N = 5$  threshold in the recent work [1] with the earlier reported results [2] establishes inaccuracy of the former's resonance parameters [1] for the higher lying states. We arrange our resonance energies in Fig. 1 according to their respective series. It is seen that all the states reported in the present work and those of Ref. [2] are accounted for. The states with energies of  $-0.09525$  a.u. and  $-0.09513$  a.u. are  $5g6g$  and  $5p7p \ ^3P^e$ , respectively. It was one of these two states that was missed by Saha and Mukherjee [1]. Also, in Ref. [1], the  $5p^2 \ ^3P^e$  state was not reported.

In their work, Saha and Mukherjee [1] also presented the  $2pnp \ ^3P^e$  state energies which are much lower than the best reported results of Hilger *et al.* [3]. But Saha and

Mukherjee [1] also showed the numerical problems in their results using 1575-term wave functions. We have reoptimized the  $2pnp \ ^3P^e$  state energy with an increasing number of basis terms. In Table III, we compare the  $2p^2 \ ^3P^e$  and  $2p3p \ ^3P^e$  state energies obtained from the present calculations with available results. We have obtained the bound excited  $^3P^e$  state energies for the same set of nonlinear variational parameters in the framework of the Ritz variational principle. We use a maximum of up to 800 term basis functions for the resonance state calculations using the CCR method, 600 terms for the stabilization method, and 900 terms for the bound state calculations. Our nonrelativistic energy for the  $2p^2 \ ^3P^e$  state is determined as  $-0.710500155678339$  a.u., with uncertainty estimated in a few parts of  $10^{-13}$ . Our present value is comparable with the results  $-0.71050015567833$  a.u., the value reported by Hilger *et al.* [3]. Saha and Mukherjee [1] reported a much lower value of  $-0.71050016521526$  a.u. But because of a convergence problem, they could only claim the uncertainty of their results in the order of  $10^{-7}$  a.u. As for the  $2p3p \ ^3P^e$  state, we determine the nonrelativistic energy as  $-0.567812898725396$  a.u., with uncertainty estimated in a few parts of  $10^{-12}$  a.u. Our energy is also lower than  $-0.56781289872515$  a.u., as reported in Ref. [3]. Again in Ref. [1], a much lower value of  $-0.56781289980706$  a.u. was reported, but with a much larger uncertainty of  $10^{-7}$  a.u. We have used the same set of nonlinear parameters to show the convergence with the increasing number of terms.

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