PHYSICAL REVIEW A **80**, 022513 (2009)

# Doubly excited bound and resonance ($^3P^e$) states of helium

Jayanta K. Saha and Tapan K. Mukherjee
*Narula Institute of Technology, Agarpara, Kolkata 700 109, India*

(Received 22 April 2009; published 25 August 2009)

Highly precise energy values for the first 14 $^3P^e$ bound states of helium arising out of two electrons having equal azimuthal quantum number are being calculated by using Ritz variational method. The present calculated upper bound energies are lowest yet obtained. Resonance energies and widths for a wide range of resonance states ($^3P^e$) of helium below $N=3-5$ ionization threshold of He$^+$ have also been evaluated by using stabilization method. The present resonance parameters for the region below $N=3-5$ ionization threshold of He$^+$ are in excellent agreement with the few available accurate theoretical results. Moreover in the present paper, the resonance parameters of $^3P^e$ resonance states below $N=6$ and 7 ionization thresholds of He$^+$ are also reported.

DOI: 10.1103/PhysRevA.80.022513 PACS number(s): 31.15.vj, 31.15.xt

## I. INTRODUCTION

Doubly excited states (DESs) for neutral helium have drawn the attention of a large number of theoreticians as they provide a fundamental testing ground for the accuracy of the theoretical treatment. On the basis of stability, DES can be classified into two general groups, as bound and resonance states, depending on the angular momentum coupling scheme and parity conservation rule [1]. This exactly quantized DES decay to the lower excited states through electronic dipole interaction giving rise to sharp spectral lines. Among such nonautoionizing DES, $2p^2(^3P^e)$ state is the lowest lying $P$ state of even parity. Compton and Boyce [2], Kruger [3], and Whiddington and Priestley [4] are the pioneers to observe such exactly quantized DES of helium. The existence of such bound states was confirmed by a series of experiments done by Tech and Ward [5], Berry *et al.* [6], and Baltzer and Karlsson [7]. It is well known that, in order to calculate accurate energy values of different singly and doubly excited states, electron correlation plays a significant role and the difference among various theoretical approaches [1,8–15] lies in the method of incorporating electron correlation of DES of two electron atoms. To incorporate angular correlation effect in the Ritz variational method for calculating the energy values of different singly and doubly excited states, the best way is to expand the trial wave function in Hylleraas basis and effort was given by many workers [16–22] to evaluate precise energy values for doubly excited states of helium using Hylleraas basis. Accurate values of the DES energy levels help us to diagnose lines observed in solar corona [23], high temperature plasma [24], and plasma diagnostics [25–27]. Hilger *et al.* [17] obtained so far the best energy values for the first nine $^3P^e$ state of helium due to two $p$ electrons. In the present paper, we have performed an extensive calculation with 1575 terms in Hylleraas basis function for evaluating the energy values of first 14 bound $^3P^e$ states of helium arising from two $p$ electrons below $N=2$ ionization threshold of He$^+$.

Different theoretical approaches [11–15,28] have been proposed to understand the internal structure of resonances in the isoelectronic sequence of helium. Stabilization method provides a fast and efficient method to calculate the positions and widths of DES for heliumlike systems. The development of stabilization method to investigate atomic resonances is the outcome of a long drawn struggle. Hazi and Taylor [29,30] are the pioneers to introduce stabilization method almost four decades ago for analyzing resonance states arising due to the elastic scattering from a one-dimensional model potential containing a barrier. In the beginning only the resonance positions, not the widths, were estimated by using stabilization method for different atomic systems [31–33]. Several methods were adopted for calculating the width of resonance states. Macias and Riera [34] and Lefebvre [35] calculated the width of an isolated moderately broad shaped resonance by using stabilization method where the knowledge of wave function is needed. McCurdy and McNutt [36], Simons [37], and Isaacson and Truhlar [38] calculated the widths of resonance states by using analytic continuation of the energy in the complex plane. Hazi and Taylor [29,30], Maier *et al.* [39], and Lefebvre [40] calculated the width of resonance states by using arguments about the asymptotic form of the wave function. It requires almost 23 years after the pioneering work of Hazi and Taylor [29] when Mandelshtam *et al.* [41] put forward an elegant and simple method of calculating the width of resonance states by evaluating the density of resonance states $\rho(E)$ from the stabilization diagram. This novel alternative approach [41] does not need the wave functions [34,35] nor does it require the use of complex analytic continuation [36–38] or the asymptotic form of the wave functions [29,30,39,40]. Muller *et al.* [42] successfully modified this approach [41] to evaluate the resonance parameters of doubly excited $S$ states of helium. A detailed list of references of synchrotron and laser experiments as well as the theoretical works for understanding the internal structure of resonances in the isoelectronic sequence of helium was given by Muller *et al.* [42]. Later Tan and Ho [43] applied this modified approach for the calculation of resonance positions and widths of $2s^2(^1S^e)$ and $2s2p(^3P^o)$ states of H$^-$. Recently a series of calculation was done by Kar and Ho [44–46] to investigate the effect of Debye plasma on the widths of different doubly excited resonance states of helium adopting the modified version of stabilization method as given by Mandelshtam *et al.* [41] and Muller *et al.* [42]. To the best of our knowledge, except $2s^2(^1S^e)$ state [44], there was no calculation for the evaluation of resonance parameters of doubly excited states of helium using modified version of stabilization method in Hylleraas basis. Recently Kar and Ho [45] mentioned that Hylleraas type basis has led to technical difficulties that need to be overcome while they have been investigating the effect of weakly coupled plasma on ${}^{1,3}P^e$ bound and resonance states arising from two electrons having same azimuthal quantum number of helium. Under such circumstances, adopting Hylleraas basis set a rigorous calculation using stabilization method is necessary to evaluate the resonance parameters of $P$ states of helium arising from two electrons having same azimuthal quantum number. The aim of this paper is to show that adopting sufficient number of terms in the Hylleraas basis set, the modified version of stabilization method as developed by Mandelshtam *et al.* [41] and Muller *et al.* [42] can produce precise values for the positions and widths of a large number of ${}^3P^e$ resonance states arising from two electrons having equal azimuthal quantum number below $N=3-7$ ionization threshold of He$^+$.

## II. METHOD

The reduction in the nine-dimensional variational equation to three-dimensional one for two electrons in the field of a nucleus is an immediate consequence of translational and rotational symmetry of the field [47,48]. Exploiting translational invariance of the Hamiltonian, the nine-dimensional variational equation reduces to six-dimensional one. Among the six coordinates, three coordinates are the sides of the triangle formed by the three particles, i.e., the two electrons, the fixed nucleus, and the other three coordinates are the three Eulerian angles defining the orientation of this triangle in space. For any ${}^3P^e$ state of even parity arising from two electrons having equal azimuthal quantum number, the variational equation [18] is given by

$$\delta\int\left[\left(\frac{\partial f_1^0}{\partial r_1}\right)^2+\left(\frac{\partial f_1^0}{\partial r_2}\right)^2+(r_1^{-2}+r_2^{-2})\left(\frac{\partial f_1^0}{\partial\theta_{12}}\right)^2+(r_1^{-2}+r_2^{-2})\times(f_1^0)^2\frac{1}{\sin^2\theta_{12}}+2(V-E)(f_1^0)^2\right]dV_{r_1,r_2,\theta_{12}}=0. \qquad (1)$$

Subject to the normalization condition,

$$\int (f_1^0)^2 dV_{r_1,r_2,\theta_{12}}=1. \qquad (2)$$

The symbols in Eqs. (1) and (2) are the same as in Ref. [47]. We used atomic unit throughout. The correlated wave function is given by

$$\begin{aligned} f_1^0(r_1,r_2,r_{12}) &= \sum_{i=1}^{9}\eta_i(1)\eta_i(2)\times\left[\sum_{l>0}\sum_{m>0}\sum_{n\geq 0}C_{lmn}r_1^l r_2^m r_{12}^n\sin\theta_{12}+\text{exchange}\right]\\ &+\sum_{i=1}^{9}\sum_{\substack{j=1\\ i<j}}^{9}\left[\eta_i(1)\eta_j(2)\sum_{l>0}\sum_{m>0}\sum_{n\geq 0}C_{lmn}r_1^l r_2^m r_{12}^n\sin\theta_{12}+\text{exchange}\right], \end{aligned} \qquad (3)$$

where

$$\eta_j(i)\sim e^{-\sigma_j r_i} \qquad (4)$$

and $\sigma$'s are the nonlinear parameters. The different $\sigma$'s in the Slater type orbitals incorporate the effect of radial correlation in the wave function. The wave functions can be squeezed or can be made more diffuse by changing the nonlinear parameter ($\sigma$) values. Following the prescription of Bylicki [49], present calculation includes nine different $\sigma$ values which form a geometrical sequence: $\sigma_i=\sigma_{i-1}\gamma^{-1}$, where $\gamma$ is the geometrical ratio. The bound state energy eigenvalues are determined by the matrix diagonalization method. The preliminary guess for the values of nonlinear parameters ($\sigma$) starts from the values of $\sigma$ obtained by Mukherjee and Mukherjee [18] where the $\sigma$'s are optimized by using Nelder-Mead procedure [50] while calculating the energy of $2p^2({}^3P^e)$ state of helium in triple exponent Hylleraas basis set. Repeated diagonalization of the Hamiltonian matrix in the Hylleraas basis set of 1575 parameters is done in the present work for different values of $\gamma$. It is found that $\sigma_1=2.69$ and $\gamma=1.4$ for the first set of nine nonlinear parameters give reasonable accurate energy values of the first nine $2pnp({}^3P^e)$ bound states of helium in one-shot diagonalization. We compute first 250 energy eigenroots for 600 different values of $\gamma$ ranging from 1.4 to 4.2. The lowest $\sigma$ value of any set differs from that of the previous one by 0.001 keeping the highest $\sigma$ value fixed at 2.69 for all the sets. All calculations are carried out in quadruple precession.

The plot of each energy eigenroots versus $\gamma$ produces the stabilization diagram. The density of resonance states is calculated from the stabilization diagram by taking the inverse of tangent at different points near the stabilization plateau for each energy eigenroot. The plot of calculated density of resonance states versus energy for each eigenroot is fitted to a Lorentzian profile. The best fit, i.e., with the least chi square ($\chi^2$) and the square of correlation near unity gives the desired energy ($E_r$) and width ($\Gamma$) of the resonance state. All plots and fitting procedure are carried out by using MICROCAL ORIGIN 6.0 software package.

## III. RESULTS AND DISCUSSIONS

The present calculated bound state energy eigenvalues ($-E$) and corresponding values of $\gamma$ for a series of $2pnp({}^3P^e)$ ($n=2-15$) states of helium for different total numbers of terms ($M$) in the wave function are given in Table I. The electronic configuration of ${}^3P^e$ states below $N=2$ ionization threshold of He$^+$ is given in the first column of Table I. So far the best results as obtained by Hilger *et al.* [17] for first nine available energy eigenvalues of ${}^3P^e$ states of helium are given in the last column of Table I for a comparison with the present calculated values. From this comparison, it is evident that the present energy eigenvalues for each of the first nine ${}^3P^e$ states are lower than those of Hilger *et al.* [17]. Hence the present energy eigenvalues of ${}^3P^e$ states can be set as benchmark for the future.

Tech and Ward [5] observed the sharp line in the far ultraviolet region with wave number 312 214.52 ± 0.97 cm$^{-1}$ corresponding to a wavelength of 320.2926 ± 0.001 Å. The present calculated wave number of 312 217.16 cm$^{-1}$ for the

TABLE I. Nonrelativistic energy eigenvalues ($-E$) a.u. of $^3P^e$ bound states of helium below $N=2$ ionization threshold of He$^+$. The maximum uncertainty of the calculated energy value is of the order of $10^{-7}$ a.u.

| Electronic Configuration | Present | | | | | | Ref. [16] |
|---|---|---|---|---|---|---|---|
| | $M=450$ | | $M=980$ | | $M=1575$ | | |
| | $\gamma$ | $-E$ (a.u.) | $\gamma$ | $-E$ (a.u.) | $\gamma$ | $-E$ (a.u.) | |
| $2p^2$ | 1.56017784 | 0.71050015567829 | 1.76055080 | 0.71050015568253 | 1.62900430 | 0.71050016521526 | 0.71050015567833 |
| $2p3p$ | 1.61441161 | 0.56781289872514 | 1.76370875 | 0.56781289872861 | 1.74668106 | 0.56781289980706 | 0.56781289872515 |
| $2p4p$ | 1.71909703 | 0.53586718872554 | 1.70541976 | 0.53586718880443 | 1.72757272 | 0.53586718904464 | 0.53586718876821 |
| $2p5p$ | 1.86155583 | 0.52225457200884 | 1.63764653 | 0.52225457570739 | 1.60240773 | 0.52225457591426 | 0.52225457570723 |
| $2p6p$ | 2.03129873 | 0.51516012584016 | 1.64878005 | 0.51516020385581 | 1.92474879 | 0.51516020878867 | 0.51516020385435 |
| $2p7p$ | 2.65668234 | 0.51099163326640 | 1.74819530 | 0.51099169107693 | 1.62371697 | 0.51099169141086 | 0.51099169120713 |
| $2p8p$ | | | 1.82972263 | 0.50833423581342 | 1.67102635 | 0.50833423751972 | 0.50833423750462 |
| $2p9p$ | | | 1.91505200 | 0.50653626410138 | 1.66147724 | 0.50653627911513 | 0.50653627909544 |
| $2p10p$ | | | 1.90095250 | 0.50526319344623 | 1.61954822 | 0.50526329773997 | 0.50526329773772 |
| $2p11p$ | | | | | 1.96344359 | 0.50432914367746 | |
| $2p12p$ | | | | | 1.67223944 | 0.50362326590730 | |
| $2p13p$ | | | | | 2.18508115 | 0.50319918663249 | |
| $2p14p$ | | | | | 2.41563492 | 0.50277819550078 | |
| $2p15p$ | | | | | 2.33172712 | 0.50267982512153 | |

transition $2p^2(^3P^e) \rightarrow 1s2p(^3P^o)$ of helium is in excellent agreement with the experimental result of Tech and Ward [5]. A difference of approximately 3 cm$^{-1}$ between our nonrelativistic results and that of the experiment [5] is due to relativistic and other corrections. The energy value of $-2.133\,261\,35$ a.u. for $1s2p(^3P^o)$ state of helium is taken from the experiment of Martin [51]. The conversion factor 1 a.u.$=219\,444.528$ cm$^{-1}$ is used. Baltzer and Karlsson [7] observed spectral peaks for helium at the positions of wavelengths $305.76 \pm 0.02$ and $305.60 \pm 0.05$ Å where the experimental resolution was not so precise in comparison to that of Tech and Ward [5] as is evident from the respective experimental uncertainties. However, present calculated values of 305.76 and 304.49 Å for $2p3p(^3P^e) \rightarrow 1s3p(^3P^o)$ and $2p4p(^3P^e) \rightarrow 1s4p(^3P^o)$ transitions, respectively, are in reasonable agreement with the experimental values obtained by Baltzer and Karlsson [7]. The present situation warrants precise experimental measurements of the wavelengths for the transitions $2p3p(^3P^e) \rightarrow 1s3p(^3P^o)$ and $2p4p(^3P^e) \rightarrow 1s4p(^3P^o)$. The experimental energy value of $-2.058\,197\,88$ and $-2.032\,441\,29$ a.u. for $1s3p(^3P^o)$ and $1s4p(^3P^o)$ states, respectively, of helium are taken from the Grotrian diagrams as compiled by Bashkin and Stoner, Jr. [52].

A portion of the stabilization diagram using a 1575 parameter Hylleraas basis set for $^3P^e$ states originating from two electrons of helium having same azimuthal quantum number is given in Fig. 1. First 39 energy eigenvalues in the range between $-0.725$ and $-0.225$ a.u. are shown here. The insensitivity of all the energy values with the variation in $\gamma$ for $^3P^e$ states lying below $N=2$ ionization threshold of He$^+$, i.e., below $-0.50$ a.u, confirms the fact that these are bound states as is evident from Fig. 1. The plot of energy eigenroots above $N=2$ ionization threshold of He$^+$ as shown in Fig. 1 also indicates that each energy eigenvalue changes with the change in $\gamma$. This is a consequence of the presence of resonance states between the energy range of $-0.5$ to $-0.225$ a.u., i.e., between $N=2$ and $N=3$ ionization thresholds of He$^+$. For a short range of $\gamma$ each eigenroot between $N=2$ and $N=3$ ionization thresholds of He$^+$ becomes almost flat in the vicinity of resonance states. A closer look of Fig. 1 in the energy range of $-0.35$ to $-0.225$ a.u. is able to give such flat plateau near the resonance states. This is evident in Fig. 2 where 25th to 54th energy values in the energy range of $-0.35$ to $-0.225$ a.u. are shown. The density of states $\rho(E)$ is then calculated by evaluating the inverse of the slope at $n$ number of points near the flat plateau of each energy eigenroot using the formula given by

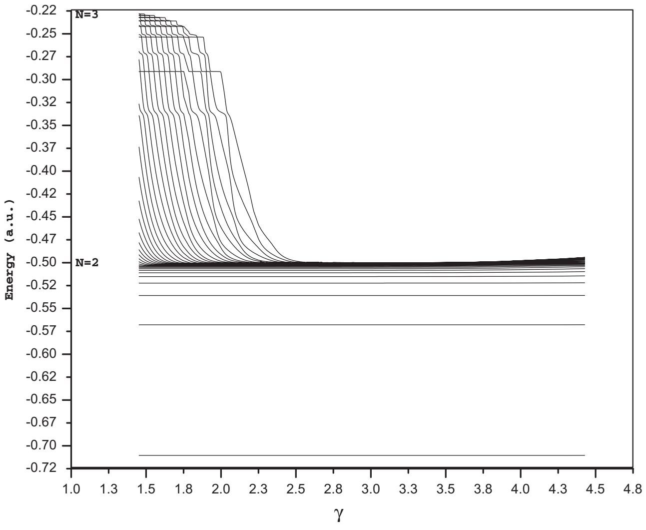

FIG. 1. Stabilization plot for the $^3P^e$ states of helium.

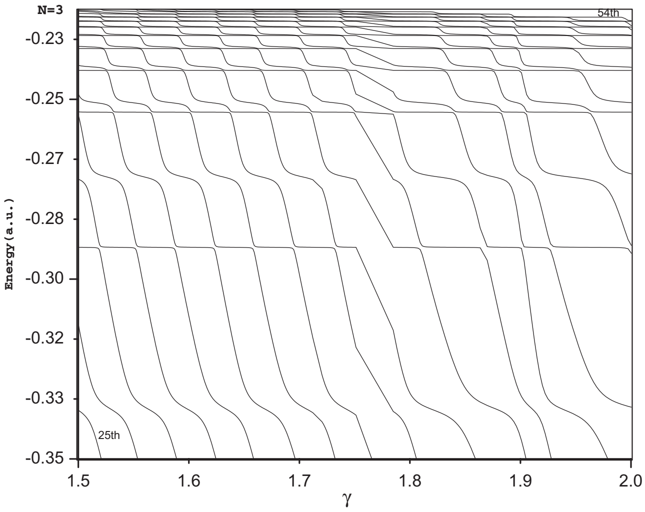

FIG. 2. Enlarged view of a portion of the stabilization plot for the $^3P^e$ states of helium between the energy interval of −0.35 to −0.225 a.u., where the eigenroots ranging from 25 to 54 are shown.

$$\rho_n(E) = \left| \frac{\gamma_{i+1} - \gamma_{i-1}}{E_n(\gamma_{i+1}) - E_n(\gamma_{i-1})} \right|_{E_n(\gamma_i)=E_i}. \tag{5}$$

The calculated density of resonance states $\rho_n(E)$ is then fitted to the following Lorentzian form:

$$\rho_n(E) = y_0 + \frac{A}{\pi} \frac{\Gamma/2}{(E - E_r)^2 + (\Gamma/2)^2}, \tag{6}$$

where $y_0$ is the baseline background, $A$ is the total area under the curve from the baseline, $E_r$ gives the position of the center of the peak of the curve, and $\Gamma$ represents the full width of the peak of the curve at half height. Among different fitting curves for each eigenroot corresponding to a particular resonance state, the fitting curve with least $\chi^2$ and the square of correlation closer to unity leads to the desired resonance energy ($E_r$) and width ($\Gamma$). For example, from the stabilization plot (Fig. 2) for the first $^3P^e$ resonance state below $N=3$ ionization threshold of He$^+$, we have calculated the inverse of the slope by using Eq. (5) at different points near the flat plateau of 29th eigenvalues in the interval of $\gamma=1.61-1.64$. The corresponding fitted curve is obtained by using Eq. (6) and is shown in Fig. 3. The circles in Fig. 3 are the calculated values of $\rho_n(E)$, while the solid line corresponds to the fitted curve. Repeated calculations of $\rho_n(E)$ near the flat plateau of each of the eigenroot for first $^3P^e$ resonance state resulted Lorentzian fitted curve similar to that of Fig. 3. Among all this fitting curve, we have found that 29th eigenroot corresponds to the best fit and from which $E_r=-0.336\,07$ a.u. and $\Gamma=0.004\,536\,7$ a.u. are obtained.

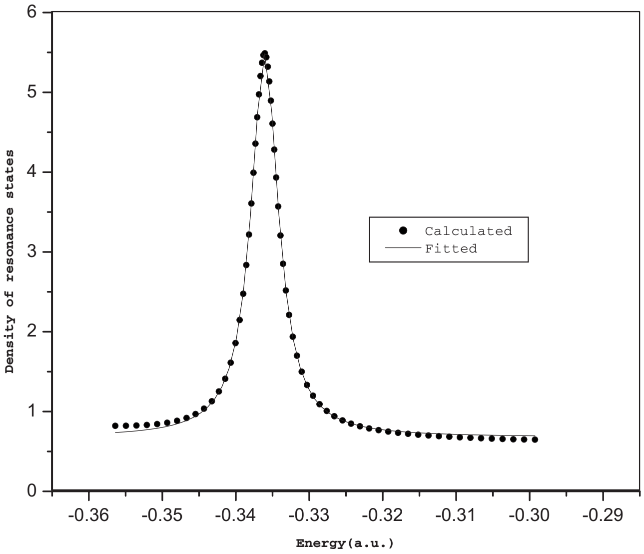

FIG. 3. Calculated density (circles) and the fitted Lorentzian (solid line) for the first $^3P^e$ resonance state of helium below $N=3$ ionization threshold of He$^+$.

TABLE II. Convergence behavior for the resonance position and width (in a.u.) of $^3P^e$ resonance states below $N=3$ ionization threshold of He$^+$.

| | $M=450$ | | $M=980$ | | $M=1575$ | |
|---|---|---|---|---|---|---|
| State | $E_r$ (a.u.) | $\Gamma$ (a.u.) | $E_r$ (a.u.) | $\Gamma$ (a.u.) | $E_r$ (a.u.) | $\Gamma$ (a.u.) |
| (1) | −0.33602 | 0.00447 | −0.33607 | 0.00446 | −0.33607 | 0.00454 |
| (2) | −0.29116 | 0.00007 | −0.29116 | 0.00007 | −0.29116 | 0.00007 |
| (3) | −0.27155 | 0.00181 | −0.27156 | 0.00176 | −0.27156 | 0.00177 |
| (4) | −0.25357 | 0.00002 | −0.25357 | 0.00002 | −0.25357 | 0.00002 |
| (5) | −0.25092 | 0.00085 | −0.25095 | 0.00085 | −0.25093 | 0.00085 |
| (6) | −0.24196 | 0.00001 | −0.24196 | 0.00001 | −0.24196 | 0.00001 |
| (7) | −0.24094 | 0.00044 | −0.24095 | 0.00045 | −0.24094 | 0.00045 |
| (8) | −0.23589 | 8.1276(−6) | −0.23589 | 9.1038(−6) | −0.23589 | 9.3389(−6) |
| (9) | −0.23537 | 0.00024 | −0.23539 | 0.00025 | −0.23539 | 0.00027 |
| (10) | −0.23224 | 9.5301(−5) | −0.23227 | 7.0733(−6) | −0.23227 | 6.3229(−6) |
| (11) | −0.23187 | 0.00020 | −0.23198 | 0.00020 | −0.23198 | 0.00017 |

TABLE III. Resonance energies $-E_r$ (in a.u.) and widths $\Gamma$ (in a.u.) of doubly excited $^3P^e$ resonance states of helium below $N=3-7$ ionization threshold of He$^+$. The notation $P(-Q)$ stands for $P\times 10^{-Q}$. The uncertainty of the resonance positions and widths is given in the parenthesis.

| | $N=3$ | | | | $N=4$ | | | | $N=5$ | | | | $N=6$ | | $N=7$ | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Present | | Ref. [28] | | Present | | Ref. [28] | | Present | | Ref. [28] | | Present | | Present | |
| $^3P^e$ | $-E_r$ | $\Gamma$ | $-E_r$ | $\Gamma$ | $-E_r$ | $\Gamma$ | $-E_r$ | $\Gamma$ | $-E_r$ | $\Gamma$ | $-E_r$ | $\Gamma$ | $-E_r$ | $\Gamma$ | $-E_r$ | $\Gamma$ |
| | 0.33607 | 4.54(−3) | | | 0.19738 | 3.37(−3) | | | 0.11937 | 1.95(−3) | | | 0.07721 | 7.38(−4) | 0.05363 | 2.50(−4) |
| 1 | [5.42(−6)] | [2.0(−5)] | 0.33609 | 4.49(−3) | [5.01(−6)] | [4.70(−4)] | 0.19442 | 4.48(−3) | [1.00(−6)] | [2.11(−4)] | 0.11930 | 3.54(−3) | [6.63(−6)] | [7.00(−5)] | [6.95(−6)] | [3.00(−5)] |
| | 0.29116 | 7.00(−5) | | | 0.17878 | 4.59(−3) | | | 0.10996 | 1.85(−3) | | | 0.07079 | 9.66(−4) | 0.05190 | 5.60(−4) |
| 2 | [1.41(−8)] | [5.52(−8)] | 0.29116 | 7.00(−5) | [2.02(−6)] | [1.10(−4)] | 0.17826 | 4.81(−3) | [1.45(−6)] | [7.00(−5)] | 0.10946 | 3.12(−3) | [2.13(−6)] | [8.00(−5)] | [3.01(−6)] | [1.00(−5)] |
| | 0.27156 | 1.77(−3) | | | 0.16136 | 1.89(−3) | | | 0.10765 | 1.00(−3) | | | 0.06825 | 1.47(−3) | 0.05085 | 9.00(−5) |
| 3 | [3.24(−7)] | [1.29(−6)] | 0.27156 | 1.79(−3) | [1.00(−6)] | [5.02(−5)] | 0.16122 | 1.90(−3) | [4.04(−6)] | [1.70(−4)] | 0.10726 | 1.53(−3) | [3.01(−6)] | [2.10(−4)] | [1.37(−5)] | [5.94(−6)] |
| | 0.25357 | 2.00(−5) | | | 0.15520 | 2.70(−4) | | | 0.10299 | 2.04(−3) | | | 0.06704 | 5.50(−4) | 0.04965 | 4.00(−5) |
| 4 | [5.25(−9)] | [2.11(−8)] | 0.25357 | 2.00(−5) | [9.55(−6)] | [4.00(−5)] | 0.15518 | 2.50(−4) | [1.70(−6)] | [6.50(−4)] | 0.10210 | 2.27(−3) | [1.00(−6)] | [6.00(−5)] | [2.56(−6)] | [1.00(−6)] |
| | 0.25093 | 8.50(−4) | | | 0.15154 | 1.54(−3) | | | 0.09828 | 8.28(−4) | | | 0.06665 | 2.98(−4) | 0.04860 | 2.10(−4) |
| 5 | [3.73(−7)] | [1.68(−6)] | 0.25093 | 8.50(−4) | [4.88(−6)] | [2.03(−5)] | 0.15155 | 1.77(−3) | [2.06(−6)] | [1.00(−5)] | 0.09860 | 9.10(−4) | [4.41(−6)] | [2.00(−5)] | [5.37(−6)] | [2.00(−5)] |
| | 0.24196 | 1.00(−5) | | | 0.14808 | 1.16(−3) | | | 0.09656 | 9.06(−4) | | | 0.06545 | 5.49(−4) | 0.04752 | 5.90(−4) |
| 6 | [3.31(−9)] | [1.35(−8)] | 0.24196 | 1.00(−5) | [7.94(−6)] | [3.00(−5)] | 0.14803 | 1.05(−3) | [8.21(−6)] | [2.31(−5)] | 0.09664 | 1.37(−3) | [2.44(−6)] | [2.01(−5)] | [2.00(−6)] | [8.01(−5)] |
| | 0.24096 | 4.50(−4) | | | 0.14235 | 5.10(−4) | | | 0.09526 | 4.02(−4) | | | 0.06522 | 1.41(−4) | 0.04655 | 3.00(−5) |
| 7 | [2.64(−7)] | [1.24(−6)] | 0.24096 | 4.50(−4) | [4.36(−7)] | [1.11(−5)] | 0.1423415 | 3.30(−4) | [1.02(−5)] | [5.02(−5)] | 0.09525 | 8.85(−5) | [2.36(−6)] | [8.87(−6)] | [5.64(−7)] | [2.16(−6)] |
| | 0.23589 | 9.34(−6) | | | 0.14207 | 7.40(−4) | | | 0.09365 | 4.53(−4) | | | 0.06449 | 1.02(−5) | 0.04573 | 1.50(−4) |
| 8 | [3.15(−9)] | [1.27(−8)] | 0.23589 | 8.00(−6) | [2.01(−6)] | [8.00(−5)] | 0.142341 | 8.40(−4) | [3.22(−6)] | [2.00(−5)] | 0.09513 | 1.48(−3) | [1.10(−7)] | [5.08(−7)] | [4.27(−6)] | [2.00(−5)] |
| | 0.23539 | 2.70(−4) | | | 0.14090 | 8.00(−4) | | | 0.09166 | 6.54(−4) | | | 0.06383 | 3.04(−4) | 0.04519 | 5.00(−5) |
| 9 | [2.39(−7)] | [1.13(−6)] | | | [7.62(−6)] | [4.02(−5)] | 0.14084 | 5.70(−4) | [2.01(−5)] | [7.01(−5)] | 0.09343 | 4.10(−4) | [3.16(−6)] | [2.00(−5)] | [9.24(−7)] | [4.14(−6)] |
| | 0.23227 | 6.32(−6) | | | 0.13742 | 5.80(−4) | | | 0.09112 | 7.37(−4) | | | 0.06358 | 6.85(−6) | 0.04484 | 2.20(−4) |
| 10 | [1.81(−9)] | [7.47(−9)] | | | [7.41(−6)] | [2.00(−5)] | 0.13729 | 6.10(−4) | [7.92(−6)] | [3.07(−5)] | 0.09151 | 9.40(−4) | [2.97(−7)] | [4.15(−7)] | [5.16(−6)] | [4.00(−5)] |
| | 0.23198 | 1.70(−4) | | | 0.13716 | 1.10(−4) | | | 0.09072 | 3.45(−5) | | | 0.06272 | 6.77(−7) | 0.04409 | 5.50(−4) |
| 11 | [2.77(−7)] | [1.32(−6)] | | | [1.03(−6)] | [4.18(−6)] | 0.13715 | 1.10(−4) | [8.05(−8)] | [3.24(−7)] | 0.09110 | 8.50(−4) | [4.17(−7)] | [4.82(−8) | [4.21(−7)] | [2.35(−5)] |
| | 0.22992 | 4.49(−6) | | | 0.13655 | 4.80(−4) | | | 0.09026 | 2.54(−4) | | | 0.06187 | 3.47(−4) | 0.04337 | 3.30(−4) |
| 12 | [1.78(−9)] | [7.30(−9)] | | | [7.44(−6)] | [2.00(−5)] | | | [7.78(−6)] | [4.01(−5)] | 0.09072 | 4.20(−5) | [6.00(−5)] | [2.20(−5)] | [1.01(−5)] | [4.00(−5)] |
| | 0.22974 | 1.10(−4) | | | 0.13405 | 4.00(−5) | | | 0.08908 | 5.99(−4) | | | 0.06115 | 2.51(−5) | | |
| 13 | [1.48(−7)] | [7.19(−7)] | | | [2.37(−7)] | [8.56(−7)] | | | [2.14(−5)] | [1.14(−5)] | | | [1.74(−7)] | [7.80(−7)] | | |
| | 0.22831 | 3.25(−6) | | | 0.13375 | 1.80(−4) | | | 0.08850 | 1.99(−5) | | | 0.06075 | 1.84(−4) | | |
| 14 | [1.39(−9)] | [5.66(−9)] | | | [7.84(−6)] | [3.00(−5)] | | | [6.85(−7)] | [2.65(−6)] | | | [1.01(−6)] | [5.00(−5)] | | |

TABLE III. (*Continued.*)

| | $N=3$ | | | | $N=4$ | | | | $N=5$ | | | | $N=6$ | | $N=7$ | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Present | | Ref. [28] | | Present | | Ref. [28] | | Present | | Ref. [28] | | Present | | Present | |
| $^3P^e$ | $-E_r$ | Γ | $-E_r$ | Γ | $-E_r$ | Γ | $-E_r$ | Γ | $-E_r$ | Γ | $-E_r$ | Γ | $-E_r$ | Γ | $-E_r$ | Γ |
| | 0.22819 | 8.00(−5) | | | 0.13202 | 2.69(−4) | | | 0.08810 | 1.38(−4) | | | 0.06028 | 3.26(−4) | | |
| 15 | [1.39(−7)] | [6.22(−7)] | | | [6.91(−6)] | [2.00(−5)] | | | [5.97(−7)] | [2.10(−6)] | | | [2.68(−6)] | [1.02(−5)] | | |
| | 0.22716 | 2.41(−6) | | | 0.13182 | 1.78(−4) | | | 0.08744 | 2.20(−5) | | | 0.05973 | 4.69(−4) | | |
| 16 | [1.72(−9)] | [7.02(−9)] | | | [3.30(−6)] | [1.01(−5)] | | | [6.61(−6)] | [2.23(−6)] | | | [2.00(−6)] | [9.00(−5)] | | |
| | 0.22707 | 7.00(−5) | | | 0.13077 | 2.41(−4) | | | 0.08696 | 2.03(−4) | | | 0.05913 | 5.34(−4) | | |
| 17 | [1.46(−7)] | [7.44(−7)] | | | [2.18(−6) | [7.93(−6)] | | | [9.16(−6)] | [3.00(−5)] | | | [7.53(−6)] | [3.00(−5)] | | |
| | 0.22631 | 1.65(−6) | | | 0.13062 | 2.70(−4) | | | 0.08602 | 3.59(−4) | | | 0.05774 | 3.37(−4) | | |
| 18 | [9.42(−8)] | [4.30(−8)] | | | [3.12(−6)] | [1.02(−5)] | | | [4.01(−6)] | [2.20(−5)] | | | [2.01(−6)] | [7.11(−5)] | | |
| | 0.22624 | 5.00(−5) | | | 0.13047 | 1.03(−4) | | | 0.08593 | 1.55(−4) | | | 0.05632 | 2.54(−4) | | |
| 19 | [2.03(−7)] | [9.88(−7)] | | | [2.14(−6)] | [7.33(−6)] | | | [4.17(−6)] | [2.00(−5)] | | | [6.81(−6)] | [4.00(−5)] | | |
| | 0.22565 | 6.86(−6) | | | 0.12952 | 4.81(−5) | | | 0.08543 | 2.24(−4) | | | | | | |
| 20 | [9.23(−8)] | [4.01(−7)] | | | [4.08(−6)] | [1.11(−7)] | | | [1.63(−6)] | [5.45(−6)] | | | | | | |
| | 0.22561 | 4.00(−5) | | | 0.12879 | 2.80(−5) | | | 0.08491 | 2.35(−4) | | | | | | |
| 21 | [2.05(−7)] | [9.97(−7)] | | | [1.19(−7)] | [7.21(−7)] | | | [7.91(−6)] | [3.00(−5)] | | | | | | |
| | 0.22514 | 2.00(−5) | | | 0.12764 | 5.48(−5) | | | | | | | | | | |
| 22 | [1.65(−7)] | [7.26(−7)] | | | [2.91(−6)] | [9.06(−6)] | | | | | | | | | | |

In Table II, the convergence behavior of first 11 $^3P^e$ resonance states of helium below $N=3$ ionization threshold of He$^+$ is shown. It is clear from Table II that the values of resonance parameters are quite stable when the numbers of terms ($M$) in the wave function are increased from 450 to 980 and 980 to 1575. Resonance energy ($E_r$) and width ($\Gamma$) of a wide range of $^3P^e$ states between $N=2$ and $N=7$ ionization thresholds of He$^+$ using 1575 terms in the Hylleraas basis set are summarized in Table III. Few available precise resonance parameter values obtained by Ho and Bhatia [28] by using complex coordinate rotation method are included in Table III for a comparison with the present one. It is evident from the comparison that the values of the present resonance parameters below $N=3$ ionization threshold of He$^+$ are in excellent agreement with that of Ho and Bhatia [28]. It is interesting to note that the width of $^3P^e$ states below $N=3$ ionization threshold of He$^+$ decreases appreciably for alternate even number of states. We are of the same opinion as of Ho and Bhatia [28] that these even numbers of states, i.e., $^3P^e$ (2), $^3P^e$ (4), $^3P^e$ (5), etc., below $N=3$ ionization threshold of He$^+$ are due to the $3dnd$ configuration while the odd numbers of states, i.e., $^3P^e$ (1), $^3P^e$ (3), $^3P^e$ (5), etc., are due to $3pnp$ configuration. It is also clear from Table III that the present calculated resonance energies ($E_r$) and widths ($\Gamma$) below $N=4$ and $N=5$ ionization thresholds of He$^+$ are in reasonable agreement to that of Ho and Bhatia [28] with few exceptions. For example, according to Ho and Bhatia [28] the seventh and eighth resonance positions ($E_r$) below $N=4$ occur at $-0.142\,341\,5$ and $-0.142\,341$ a.u., respectively. The degeneracy of seventh and eighth resonance states below $N=4$ as obtained by Ho and Bhatia [28] is being removed in the present calculation. Again the resonance energy of $-0.095\,13$ a.u. for eighth resonance state below $N=5$ as obtained by Ho and Bhatia [28] is not in conformity with the present one. For a better understanding, the present calculated values and that of Ho and Bhatia [28] for the resonance position ($E_r$) below $N=5$ are shown side by side in Fig. 4. The position of eighth resonance state below $N=5$ as obtained by Ho and Bhatia [28] almost coincides with that of seventh resonance state as is evident from Fig. 4. The sudden decrease in the gap between seventh and eighth resonance states below $N=5$ as obtained by Ho and Bhatia [28] does not match with their trend of spacing between the energy levels. The present calculated resonance positions for 8th to 11th states below $N=5$ are in reasonable agreement with that of 9th to 12th states of Ho and Bhatia [28], respectively, as is evident from Table III and Fig. 4. It also appears from Table III that the present method yields more number of resonance states below $N=3-5$ than that of complex coordinate rotation method as used by Ho and Bhatia [28]. This is a clear advantage of the stabilization method over the complex coordinate rotation method.

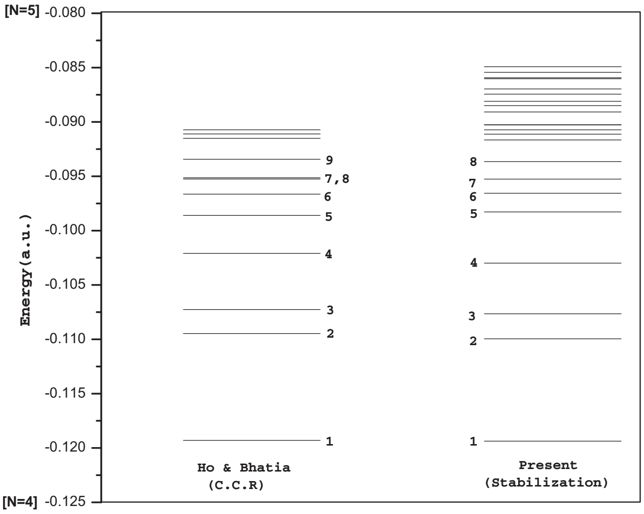

FIG. 4. Energy level diagram of resonance states below $N=5$ ionization threshold of He$^+$.

In conclusion it can be said that the use of stabilization method as developed by Mandelshtam *et al.* [41] and Muller *et al.* [42] with sufficient number of terms in the Hylleraas basis set yields accurate resonance parameters for a wide range of resonance states of helium.

## ACKNOWLEDGMENTS

Authors are thankful to the Department of Atomic Energy, BRNS, Government of India for the financial assistance under Grant No. 2007/37/59/BRNS/436. Authors express gratitude to Professor P. K. Mukherjee, Department of Spectroscopy, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700 034 for critical reading of the paper. The authors express heartfelt thanks to Professor M. Bylicki, Instytut Fizyki, Uniwersytet MikoÃlaja Kopernika, Grudziadzka 5, PL-87-100 Torun, Poland for stimulating discussions. We are also thankful to Rahul Kumar Sharma, St. Xaviers College, Kolkata for computational assistance.

---

[1] G. W. F. Drake and A. Dalgarno, Phys. Rev. A **1**, 1325 (1970).
[2] K. T. Compton and J. C. Boyce, J. Franklin Inst. **205**, 497 (1928).
[3] P. G. Kruger, Phys. Rev. **36**, 855 (1930).
[4] R. Whiddington and H. Priestley, Proc. R. Soc. London, Ser. A **145**, 462 (1934).
[5] J. L. Tech and J. F. Ward, Phys. Rev. Lett. **27**, 367 (1971).
[6] H. G. Berry, I. Martinson, L. J. Curtis, and L. Lundin, Phys. Rev. A **3**, 1934 (1971).
[7] P. Baltzer and L. Karlsson, Phys. Rev. A **38**, 2322 (1988).
[8] E. Holoien, J. Chem. Phys. **29**, 676 (1958); Phys. Norv. **1**, 53 (1961).
[9] K. Aashamar, University of Oslo Report No. 35, 1969 (unpublished).
[10] D. R. Herrick and O. Sinanoglu, Phys. Rev. A **11**, 97 (1975).
[11] W. Shearer-Izumi, At. Data Nucl. Data Tables **20**, 531 (1977).
[12] H. Bachau, F. Martin, A. Riera, and M. Yanez, At. Data Nucl. Data Tables **48**, 167 (1991).

[13] L. Lipsky, R. Anania, and M. J. Connely, At. Data Nucl. Data Tables **20**, 127 (1977).
[14] H. W. Van der Hart and J. E. Hansen, J. Phys. B **26**, 641 (1993).
[15] P. M. Becker and J. S. Dahler, Phys. Rev. **136**, A73 (1964).
[16] A. K. Bhatia, Phys. Rev. A **2**, 1667 (1970).
[17] R. Hilger, Hans-Peter Merckens, and H. Kleindienst, Chem. Phys. Lett. **262**, 400 (1996).
[18] T. K. Mukherjee and P. K. Mukherjee, Phys. Rev. A **69**, 064501 (2004).
[19] A. N. Sil, T. K. Mukherjee, and P. K. Mukherjee, Chem. Phys. Lett. **406**, 279 (2005).
[20] S. Bhattacharyya, A. N. Sil, T. K. Mukherjee, and P. K. Mukherjee, J. Chem. Phys. **123**, 196102 (2005).
[21] S. Bhattacharyya, A. N. Sil, T. K. Mukherjee, and P. K. Mukherjee, J. Chem. Phys. **126**, 011104 (2007).
[22] S. Bhattacharyya, T. K. Mukherjee, J. K. Saha, and P. K. Mukherjee, Phys. Rev. A **78**, 032505 (2008).
[23] A. B. C. Walker, Jr. and H. R. Rugge, Astrophys. J. **164**, 181 (1971); G. A. Doschek, J. F. Meckins, R. W. Kreplin, T. A. Chubb, and A. Friedman, *ibid.* **164**, 165 (1971).
[24] N. J. Peacock, R. J. Speer, and M. G. Hobby, J. Phys. B **2**, 798 (1969); A. H. Gabriel and C. Jordon, Nature (London) **221**, 947 (1969).
[25] T. Fujimoto and T. Kato, Astrophys. J. **246**, 994 (1981), and references therein.
[26] A. N. Sil, S. Bhattacharyya, and P. K. Mukherjee, Int. J. Quantum Chem. **107**, 2708 (2007), and references therein.
[27] S. Kar and Y. K. Ho, Int. J. Quantum Chem. **106**, 814 (2005) and references therein.
[28] Y. K. Ho and A. K. Bhatia, Phys. Rev. A **47**, 2628 (1993).
[29] A. U. Hazi and H. S. Taylor, Phys. Rev. A **1**, 1109 (1970).
[30] M. F. Fels and A. U. Hazi, Phys. Rev. A **4**, 662 (1971).
[31] E. Holoien and J. Midtdal, J. Phys. B **3**, 592 (1970).
[32] R. J. Drachman and S. K. Houton, Phys. Rev. A **14**, 894 (1976).
[33] Y. K. Ho, Phys. Rev. A **19**, 2347 (1979).
[34] A. Macias and A. Riera, Phys. Lett. **103A**, 377 (1984).
[35] R. Lefebvre, J. Phys. B **21**, L709 (1988).
[36] C. W. McCurdy and J. F. McNutt, Chem. Phys. Lett. **94**, 306 (1983).
[37] J. Simons, J. Chem. Phys. **75**, 2465 (1981).
[38] A. D. Isaacson and D. G. Truhlar, Chem. Phys. Lett. **110**, 130 (1984).
[39] C. H. Maier, L. S. Cederbaum, and W. Domcke, J. Phys. B **13**, L119 (1980).
[40] R. Lefebvre, J. Phys. Chem. **89**, 4201 (1985).
[41] V. A. Mandelshtam, T. R. Ravuri, and H. S. Taylor, Phys. Rev. Lett. **70**, 1932 (1993).
[42] J. Muller, X. Yang, and J. Burgdorfer, Phys. Rev. A **49**, 2470 (1994).
[43] S. S. Tan and Y. K. Ho, Chin. J. Phys. (Taipei) **35**, 701 (1997).
[44] S. Kar and Y. K. Ho, Chem. Phys. Lett. **402**, 544 (2005).
[45] S. Kar and Y. K. Ho, J. Phys. B **40**, 1403 (2007).
[46] S. Kar and Y. K. Ho, Int. J. Quantum Chem. **108**, 1491 (2008).
[47] T. K. Mukherjee and P. K. Mukherjee, Phys. Rev. A **50**, 850 (1994).
[48] T. K. Mukherjee and P. K. Mukherjee, Phys. Rev. A **51**, 4276 (1995).
[49] M. Bylicki, J. Phys. B **30**, 189 (1997).
[50] J. A. Nelder and R. Mead, Comput. J. **7**, 308 (1965).
[51] W. C. Martin, J. Res. Natl. Bur. Stand., Sect. A **64**, 19 (1960).
[52] S. Baskin and J. O. Stoner, Jr., *Atomic Energy Levels and Grotrian Diagrams I* (North-Holland, Amsterdam, 1975).