# $2s^2 2p\ ^2P^o$ triply excited state of $He^-$

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The triply excited $2s^2 2p\ ^2P^o$ state of $He^-$ is studied by using the saddle-point complex-rotation method. The energy and Auger width of this resonance are calculated. Relativistic corrections are evaluated with the first-order perturbation theory, and the mass-polarization effect is also included. The partial Auger widths are calculated for the individual open channels. The total width is obtained by coupling the important open channels and summing over the other channels. These results are compared with the theoretical and experimental data in the literature. [S1050-2947(98)05909-5]

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Since the 1960s, the $He^-$ spectrum has served as a testing ground for theoretical as well as experimental methods for the study of resonance. The triply excited $2s^2 2p\ ^2P^o$ was observed in many experiments [1–7]. Among these, only Quéméner *et al.* [3] and Marchand [5] measured the resonance width. The results are $90\pm14$ and $90\pm200$ meV, respectively. At the same time, the energy of this resonance was also calculated by using stabilization [8,9], state-specific [10], close-coupling [11], and truncated diagonalization [12] methods. In spite of many experimental and theoretical studies of $2s^2 2p\ ^2P^o$, accurate width for this resonance was still lacking.

Recently, the advances of the synchrotron technology have stimulated considerable experimental and theoretical interest in the study of triply excited atoms. More effective theoretical methods for calculating the triply excited state, such as Feshbach projection [13], complex-coordinate rotation [14], *R*-matrix [15,16], and saddle-point complex-rotation [17–19] methods have been developed. The saddle-point complex-rotation method has been applied to calculate the resonance energy and Auger width for triply excited lithium [17,20,21]. Their results agree excellently with high-precision experiments [15,22]. For $He^-$ $2s^2 2p\ ^2P^o$, Bylicki and Nicolaides have calculated the energy and the total width using Feshbach projection and complex-coordinate rotation methods [13,14]. The width is within the experimental width of $90\pm200$ meV [5] but it is outside of the experimental uncertainty of Quéméner *et al.* [3] at $90\pm14$ meV. There have been no partial width studies, to our knowledge, in the literature. Since width is an important physical quantity and in view of the existing discrepancy, it would be worthwhile to have other theoretical studies for partial and total width and to compare the total width result with those in the literature.

In this work, the saddle-point complex-rotation method [17–21] is used to calculate the energy and width of $He^-$ $2s^2 2p\ ^2P^o$. The closed-channel wave function is first calculated using the saddle-point variation method [18]. The radial basis functions are Slater orbitals. The angular and spin functions are the same as in Chung [17]. The linear and nonlinear parameters in the basis functions are determined in the energy optimization processes. Similar to Chung and Gou [21], open channels are removed from the wave functions by including the proper vacancy orbital. The vacancy orbital is taken as a hydrogenlike function and the nonlinear parameter $q$ in the orbital is determined in the energy maximization process [20]. This gives the saddle-point wave function $\Psi_b$ and the corresponding energy $E_b$ for the closed-channel part of the resonance. $\Psi_b$ has 526 terms and 33 angular-spin components. To improve the nonrelativistic energy $E_b$, we use the restricted-variation method [23] to saturate the functional space. The corrections to $E_b$ from many orthogonal angular-spin components are obtained by considering these components individually. The total correction from the restricted-variation calculations, $\Delta E_{\mathrm{RV}}$, is the sum of individual corrections.

To obtain the width of a resonance and the shift that comes from the interaction of the closed channel with open channels, the saddle-point complex-rotation method [19] is used. In our calculation, we have considered the $1s2s\ ^{1,3}S$, $1s2p\ ^{1,3}P$, $1s3p\ ^3P$, and $1s3d\ ^3D$ target states. The partial Auger widths for the individual open channels are calculated by including one open channel at a time. The total Auger width and the total shift are obtained by coupling the important open channels and summing the other channels. The convergence of the Auger width and shift is checked with respect to the angle of complex scaling (0.3~0.7 rad) and the variation of the nonlinear parameters in the outgoing wave function. The results show that the partial widths are stable

TABLE I. Partial widths ($\Gamma_p$) and the total width ($\Gamma$) of $2s^2 2p\ ^2P^o$ triply excited state of $He^-$ (in meV).

| $\Gamma_p$ | | | | | | | | $\Sigma\Gamma_p$ | $\Gamma$ |
|---|---|---|---|---|---|---|---|---|---|
| $1s2s\ ^3S$ | $1s2s\ ^1S$ | $1s2p\ ^3P$ | | $1s2p\ ^1P$ | | $1s3p\ ^3P$ | $1s3d\ ^3D$ | | |
| | | $+ks$ | $+kd$ | $+ks$ | $+kd$ | | | | |
| 0.66 | 12.55 | 41.26 | 3.06 | 13.13 | 0.43 | 0.42 | 0.32 | 71.83 | 68.54 |

 

TABLE II. Resonance energy, shift, relativistic and mass polarization corrections, term energy $T$, and width ($\Gamma$) of $2s^2 2p\ ^2P^o$ triply excited state of $He^-$ . All energies are in $\mu$a.u. except the term energy in eV and the width in meV.

| | |
|---|---|
| $E_b$ | −801574.4 |
| $\Delta E_{RV}$ | −96.19 |
| Shift $E_s$ | 356.3 |
| $E_{nonrel}$ | −801314.3 |
| $P^4$ and Darwin term | −35.54 |
| $e$-$e$ contact term | 0.1423 |
| Orbit-orbit interaction | 1.6881 |
| Mass polarization | 2.4652 |
| Resonance energy | −801345.5 |
| Term energy $T$ (eV) | 57.206 |
| Width (meV) | 68.54 |

to four digits in most cases. In Table I, we give the partial widths and the fully coupled width of the $2s^2 2p\ ^2P^o$ triply excited state of $He^-$.

To further improve the energy of the resonance, we include the relativistic corrections, and mass polarization effect. The relativistic corrections included in this work are the kinetic energy correction $P^4$ and the Darwin term, the electron-electron contract term, and the orbit-orbit interaction [24]. They are calculated using first-order perturbation theory. The mass-polarization operator is accurate to all orders. The total energy of the resonance is obtained by adding the nonrelativistic energy $E_{nonrel}$, relativistic corrections, and mass polarization. These results and the total Auger width are given in Table II. The energies are also expressed in terms of the term energy ($T$), which is the energy above the ground state of $He^-$. It is calculated by using −2.903 800 a.u. for the ground-state energy and the conversion factor 1 a.u.=27.209 27 eV.

Our results for the energy position and width of the $2s^2 2p\ ^2P^o$ triply excited state of $He^-$ are $E=57.206$ eV and $\Gamma=68.54$ meV. In Table III, these results are compared with the existing experimental and theoretical data. Our total width is very close to the theoretical value of 71 meV in Bylicki and Nicolaides [14] but outside of the experimental uncertainty of 90±14 meV. On the other hand, the energy of this resonance agrees excellently with the experimental data in the literature. It is within most of the experimental uncertainties, except that of Quéméner *et al.* [3].

TABLE III. The energy $T$ (in eV) and the width $\Gamma$ (in meV) of $2s^2 2p\ ^2P^o$ triply excited state of $He^-$.

| | Experimental | | | Theoretical | | |
|---|---|---|---|---|---|---|
| Ref. | $T$ | $\Gamma$ | Ref. | Method | $T$ | $\Gamma$ |
| [1] | 57.1±0.1 | | [8] | Stabilization | 57.3 | |
| [2] | 57.21±0.06 | | [10] | State specific | 57.3 | |
| [3] | 57.15±0.04 | 90±14 | [11] | Close coupling | 56.48 | 2.4 |
| [4] | 57.16±0.05 | | [12] | Trun. diag. | 57.35 | |
| [5] | 57.2±0.05 | 90±200 | [9] | Stabilization | 57.41 | |
| [6] | 57.22±0.04 | | [13] | Feshbach proj. | 57.196 | |
| [7] | 57.19±0.03 | | [14] | Com.-coor. rotation | 57.205 | 71 |
| | | | this work | Saddle-point complex-rotation | 57.206 | 68.54 |

In conclusion, using the saddle-point complex-rotation method, we have calculated the width and energy position of the $2s^2 2p\ ^2P^o$ triply excited state of $He^-$. Relativistic corrections are evaluated with the first-order perturbation theory, and the mass-polarization effect is also included. The partial Auger widths are calculated for the individual open channels. The total width is obtained by coupling the important open channels and summing over the other channels. Our resonance energy and width confirm the theoretical results obtained by Bylicki and Nicolaides [14] but deviate from the width of Quéméner *et al.* [3]. We hope our partial and total width results could be useful for future experiments.

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