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Energies and Auger widths of the triply excited states of He^{-*}

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Some triply excited states of He^- ion are studied using the saddle-point complex-rotation method. The energies and Auger widths of these resonances are calculated with the relativistic corrections and mass polarization taken into account. The total Auger width is obtained by coupling the important open channels and summing over the other channels. These results are in good agreement with other theoretical and experimental data in the literature.

Keywords: triply excited state, Auger width
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1. Introduction

The triply excited state of He^- is a highly excited four-body atomic system with all three electrons residing outside the K-shell, closeness to more than one threshold, and degeneracy with many continua. For He^- ion, the attractive Coulomb potential is absent. The formation of the resonances in He^- ion is very different from that in neutral atoms or positive ions. Therefore, it is challenging to calculate the resonance energies and Auger widths of triply excited states in He^-. The advances of the synchrotron technology have stimulated considerable experimental and theoretical interest in the study of the triply excited atoms.[1−19] Kuyatt *et al*[1] first reported the observation of the triply excited autoionizing states of He^- in an electron-scattering experiment. Many effective theoretical methods,[5−19] such as the R-matrix method,[5] many-body perturbation theory,[6] and saddle-point technique,[8−12] have been developed for calculation of the triply excited atomic states. However, to the best of our knowledge, few data have been reported for the triply excited states in He^- negative ion.

In this work, three triply excited states of He^- are studied. The relativistic energies, shift, and Auger widths are calculated using the saddle-point complex-rotation method. In the saddle-point method, the parameters of the vacancy orbital are determined in the energy maximization processes and those of the real orbital are determined in the energy optimization processes. This method is the most efficient for avoiding variational break-down and obtaining the close-channel energies of the triply excited states, showing the advantage in calculating atomic core-excited states. To find the actual resonance position, one needs to consider the interaction from the open channels. By including the open-channel continua via the complex- rotation method, the resonance parameters of the quantum system can be calculated with square integrable basis function. The comparisons are also made with other theoretical and experimental data in the literature.

2. Theory

In general, the closed-channel wavefunction of the triply excited three-electron system can be written as

$$\Psi_{\rm b}(1,2,3) = A[1-P_{1\rm s}(1)][1-P_{1\rm s}(2)] \times [1-P_{1\rm s}(3)]\psi(1,2,3), \qquad (1)$$

where A is the antisymmetrization operator. The projection operator P is given by

$$P_{1\rm s}(i) = |\phi_0(\boldsymbol{r}_i)\rangle\langle\phi_0(\boldsymbol{r}_i)|, \qquad (2)$$

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where the vacancy orbital is

$$\phi_0(\boldsymbol{r}) = N\exp(-qr), \tag{3}$$

q being a parameter determined in the energy maximization process. N is a normalization constant. The radial basis functions in $\psi(1,2,3)$ are Slater orbitals. The linear and nonlinear parameters in $\psi(1,2,3)$ are determined in the energy optimization processes. The $E_{\rm b}$ obtained from $\Psi_{\rm b}(1,2,3)$ is the saddle-point energy of the resonance.

The saddle-point wavefunction $\Psi_{\rm b}(1,2,3)$ represents the best approximation to the resonance with a real square-integrable basis set. To obtain the width using the saddle-point complex-rotation method, we write the total wavefunction as

$$\Psi(1,2,3) = \Psi_{\rm b}(1,2,3) + \sum_i A\phi_i(1,2)U_i(3), \tag{4}$$

where

$$U_i = \sum_n d_{i,n} r^n \exp(-\alpha_i r). \tag{5}$$

The $\phi_i(1,2)$ represents the two-electron open-channel target states. In this work, only those target states with at least one n=2 orbital will interact strongly with $\Psi_{\rm b}$, since $\Psi_{\rm b}$ couples with the open-channel continua via the two-electron operators. U_i represents the wavefunction of the outgoing electron. It contains the linear parameter $d_{i,n}$ and a nonlinear parameter α_i. In the complex-rotation computation, only the r in U_i is complex scaled. The LS coupling is adopted for these wavefunctions. The proper angular and spin coupling between ϕ_i and U_i to obtain the correct orbital L and M is implicitly assumed in the above equation. In the calculation, the nonlinear parameters obtained from the saddle-point calculation in $\Psi_{\rm b}(1,2,3)$ are retained, but the linear parameters are recalculated to allow for full interaction between the closed-channel and the open-channel wavefunctions. The energy from $\Psi_{\rm b}(1,2,3)$, $E - {\rm i}\Gamma/2$, gives the position and the width of the resonance. The difference, $E_{\rm s} = E - E_{\rm b}$, represents the shift from the saddle-point energy to the resonance energy due to the interaction between $\Psi_{\rm b}(1,2,3)$ and continua.

The total energy is further improved by the mass polarization and relativistic corrections. The relativistic perturbation operators are the kinetic energy correction (P^4), the Darwin term, the electron–electron contact term, and the orbit–orbit and spin–spin interactions. The relativistic perturbation operators are calculated using first-order perturbation theory and mass polarization is calculated to all order. The explicit expressions of these perturbation operators are given in Ref.[9], which will not be repeated here. The total energy becomes $E_{\rm total} = E_{\rm b} + E_{\rm s} + \Delta E_{\rm rel}$.

3. Result and discussion

In this work, three triply excited 2s2s2p ^{2}P$^{\rm o}$, 2s2p2p ^{4}P, and 2p2p2p ^{4}S$^{\rm o}$ states of He^- are studied. In Table 1, we give the total energies and term energies of these resonances. As Table 1 shows, the total energy of the resonances is obtained by adding up the saddle-point energy $E_{\rm b}$, shift $E_{\rm s}$, relativistic corrections, and mass polarization. The term energy means the energy above the ground state of He^-. It is calculated by using –2.903800a.u. for the ground-state energy and the conversion factor 1a.u.=27.20927eV. Comparison with the data in the Refs.[2–4,7,8,13–19] shows that our results are in good agreement with other theoretical results and experimental measurements. For the 2s2s2p ^{2}P$^{\rm o}$ state, our results for the energy position of this state are E=57.218eV. It is within all of the experimental uncertainties.[2–4] On the other hand, as Table 2 shows, our total width Γ=71.58 meV for this resonance is very close to the theoretical value of 71meV in Bylicki and Nicolaides.[14] For the 2p2p2p ^{4}S$^{\rm o}$ state, it cannot Coulomb-autoionize into an adjacent continuum state because in the LS coupling scheme there does not exist a degenerate ^{4}S$^{\rm o}$ continuum with the same parity and total orbital angular momentum L.

Table 1. Resonance energy, shift $E_{\rm s}$, relativistic $H_{\rm rel}$ and mass polarization corrections $H_{\rm mp}$, and term energy of the triply excited He^- resonances. All energies are in a.u., except the term energy in eV.

Resonances	$E_{\rm b}$	$E_{\rm s}$	$E_{\rm nonrel}$	$E_{\rm rel}$		$E_{\rm total}$	Term energy	Sources
				$H_{\rm mp}$	$H_{\rm rel}$			
2s2s2p ^{2}P$^{\rm o}$	–801379.0	510.87	–800868.1	1.69	–35.28	–800901.7	57.218	this work
							57.19±0.03	Exp.[2]
							57.2±0.05	Exp.[3]
							57.22±0.04	Exp.[4]
							57.812	Ref.[7]
							57.196	Ref.[13]
							57.205	Ref.[14]

Table 1 (*Continued*)

2s2p2p ^{4}P	–793259.7	252.84	–793006.9	3.29	–28.57	–793032.1	57.432	this work
							57.352	Ref.[7]
							57.420	Ref.[14]
							57.313	Ref.[15]
							57.419	Ref.[16]
2p2p2p ^{4}S^o	–723045.6		–723045.6	11.60	–16.31	–723050.3	59.337	this work
							59.562	Ref.[7]
							59.353	Ref.[8]
							59.373	Ref.[15]
							59.33	Refs.[17–19]

The partial widths, the total width and shifts of the triply excited 2s2s2p ^{2}P^o and 2s2p2p ^{4}P states of He^- are given in Table 2. To obtain the resonance position and width, open channel effects need to be considered. In the case of 2s2s2p ^{2}P^o, there are an infinite number of open channels. We noted that most of its Auger width comes from those He target-states with one of 2p and 2s electron. The total shift and width are obtained by coupling the important open channels and summing over the other channels. In this work, the Hamiltonian matrix of the open channels is not exactly diagonal. Hence, it is interesting to see whether the additive property of the width and shift still holds. For the 2s2s2p ^{2}P^o resonance, the sum of the partial widths agrees very well with the total width calculation. However, the sum of the shifts from the single channel calculations differs substantially from that of the fully coupled calculation. This suggests that one may not be able to estimate the full shift from the individual shifts. We calculated the partial widths and the branching ratio of this state. The possible main decay modes for the 2s2s2p ^{2}P^o resonance of He^- and corresponding Auger energies are

$$\begin{aligned} \text{2s2s2p } ^2\text{P}^o &\rightarrow \text{1s2s } ^1\text{S} + k\text{p} \quad (36.60\text{eV}, 17\%), \\ &\rightarrow \text{1s2p } ^1\text{P} + k\text{s} \quad (36.00\text{eV}, 18\%), \\ &\rightarrow \text{1s2p } ^3\text{P} + k\text{s} \quad (36.25\text{eV}, 57\%). \end{aligned} \tag{6}$$

The Auger branching ratios play an important role in identifying experimental spectra. The information from Table 2 should be very useful in better understanding of the observed Auger spectrum in the future.

Table 2. Shifts E_s, partial widths Γ_p, and branch ratios of the triply excited He^- resonances.

Resonances	Target states	Γ_p/meV	Branch ratio/%	E_s/a.u.
2s2s2p ^{2}P^o	1s1s ^{1}S+kp	0.09	0.1	41.13
	1s2s ^{1}S+kp	12.54	17.2	297.67
	1s2s ^{3}S+kp	0.65	0.9	40.67
	1s2p ^{1}P+ks	13.31	18.2	193.96
	+kd	0.43	0.6	26.54
	1s2p ^{3}P+ks	41.88	57.3	74.90
	+kd	3.28	4.5	38.45
	1s3p ^{3}P+ks	0.40	0.6	20.36
	others	0.55	0.8	0.02
	total	73.13		733.70
	fully coupled	71.58		510.87
		71[a)]		
2s2p2p ^{4}P	1s2p ^{3}P+kp	10.13	98.6	252.84
	1s3p ^{3}P+kp	0.14	1.4	33.61
	total	10.27		286.45
		10.3[a)]		

a) Ref.[14].

In summary, in this work, we have calculated the relativistic energies and partial widths of some triply excited states of He^- negative ion. By coupling the important open channels and summing over the other channels, we have obtained the total Auger widths of these resonances. These results are in good agreement with other theoretical and experimental data in the literature.

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