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SERIES REPORT

(Laser, Atomic and Molecular Physics)

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ABSTRACT

Near the $n = 3$ threshold of residual ion O^{7+}, the resonant photoionisation of the multicharged ion O^{6+} is considered by calculating the excitation energies, associated wavefunctions, partial and total widths of the $^1P^{(-)}$ and $^3P^{(-)}$ autoionising states. These calculations are made in the diagonalisation approximation in the LS coupling scheme. The results are compared with the available theoretical results obtained by authors using other theoretical approaches.

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Preface

The ICTP-LAMP reports consist of manuscripts relevant to seminars and discussions held at ICTP in the field of Laser, Atomic and Molecular Physics (LAMP).

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1. Introduction

The doubly-excited states of helium-like multicharged ions have been the subject of many papers in the ten last years [1-5]. The determination of the characteristics of resonant states are very important in the understanding of collisional and radiational processes which take place in hot astrophysical and laboratory plasma. In addition, the study of the doubly excited states of helium and its isoelectronic sequences is an important test case in the investigation of electron-correlation phenomenon [6-7].

From theory, only a few works have been done on the resonant states of O^{6+} converging to the n = 3 threshold of residual ion O^{7+} by Bachau [8] using the Feshbach formalism and by Bachau et al [9] using the pseudo-Feshbach method. In this energy region, in our knowledge, there is no experimental work concerning the autoionising states of O^{6+} .

In this work, we use the LS coupling approximation in the framework of the diagonalisation method, to calculate excitation energies,wavefunctions, partial and total widths of $^1P^o$ and $^3P^o$ autoionising levels converging to the n = 3 threshold of residual ion O^{7+} .

As it is well known, the description of resonant photoionisation of two-electron systems near the n = 3 threshold is a multichannel problem [10-11] where one must consider the interaction between resonances and several continua. When several transition channels are open, one of the most difficult problems in the determination of resonant characteristics consist of evaluating the contributions arising from the continuum, and especially to take into account the direct coupling between different continua.

Detailed diagonalisation calculations have been reported in previous works [11-12]. In the present paper, the diagonalisation approximation is briefly described in section 2. In section 3, are presented the results of calculation concerning the singlets and triplets autoionising configurations of O^{6+} (3ln'l') with n'=3,4,5 . A comparison is made between our results and those obtained by other theoretical calculations.

2. Theory

For two-electron, the photoionisation partial amplitude Ti(E) in terms of dipole matrix elements is defined by :

$$T_i(E) = \langle \psi_{Ei} | \hat{D} | \psi_0 \rangle$$

where $\hat{D}$ is the dipole momentum operator, ψ_0 is the initial atomic-state wavefunction and ψ_{Ei} is the wavefunction of the system ion+ photoelectron in the channel i.

In diagonalisation approximation , the final state wave function is expanded in the subspaces of close and open channels as following[11-12] :

$$\psi_{E_i}(\vec{r}_1, \vec{r}_2) = \hat{A} \sum_k \left[\psi_k(\vec{r}_1) U_{ki}(E, \vec{r}_2) \right] + \sum_\mu \wedge_\mu (E) \ \phi_\mu(\vec{r}_1, \vec{r}_2) \tag{1}$$

where $\hat{A}$ is the operator of antisymmetrisation , k represents a set of quantum numbers which characterise the system ion + photoelectron in the subspace of open channels, $U_{ki}(E, \vec{r}_2)$ is the unknown function describing the motion of the photoelectron, $\psi_k(\vec{r}_1)$ is the eigenfunction of reduced ion satisfying the relations :

$$\begin{aligned} &\langle \psi_k | \psi_{k'} \rangle = \delta_{kk'} \\ &\langle \psi_k | \hat{H} | \psi_{k'} \rangle = \varepsilon_k \delta_{kk'} + V_{kk'} \end{aligned} \tag{2}$$

The functions $\phi_\mu(\vec{r}_1, \vec{r}_2)$ are obtained by unitary transformation of the hamiltonian $\hat{H}$ in the subspace of closed channels

$$\phi_\mu(\vec{r}_1, \vec{r}_2) = \hat{A} \sum_{lm} \alpha_\mu \left[\psi_l(\vec{r}_1) \psi_m(\vec{r}_2) \right] \tag{3}$$

with the condition of diagonalisation :

$$\langle \phi_\mu | \hat{H} | \phi_\nu \rangle = E_\mu \delta_{\mu\nu} \tag{4}$$

The coefficients α_μ of the unitary transformation (3) are found by solving the system of linear algebraic equations :

$$\sum_\nu \left\{ (E_\mu - E_0) \delta_{\mu\nu} + \langle \chi_\mu | \hat{V} | \chi_\nu \rangle \right\} \alpha_\nu = 0 \tag{5}$$

Where Eo is the energy eigenvalue of the zero-order hamiltonian $\hat{H}_0$ corresponding to the eigenfunctions χ_ν defined by :

$$\chi_\nu = \hat{A} \left[\psi_l(\vec{r}_1) \ \psi_m(\vec{r}_2) \right] \tag{6}$$

The determination of the function $\psi_E(\vec{r}_1, \vec{r}_2)$ is equivalent to the calculation of the coefficients $\wedge_\mu(E)$ and $U_{k\mu}(E, \vec{r}_2)$. Detailed calculations of these coefficients and systems of equations which they satisfy have been reported by Wague[11-12]. From this work , the partial photoionisation amplitude which describes the formation of a residual ion and a photoelectron in a definite state , is defined by the following expression:

$$Ti = \langle \varphi_j(E) | \hat{D} | \psi_0 \rangle + \frac{q+i}{\varepsilon - i} \langle \phi_\mu | \hat{V} | \varphi_j(E) \rangle \times \frac{\sum_k \langle \phi_\mu | \hat{V} | \varphi_k(E) \rangle \langle \varphi_k(E) | \hat{D} | \psi_0 \rangle}{\sum_k \left| \langle \phi_\mu | \hat{V} | \varphi_k(E) \rangle \right|^2} \quad (7)$$

In (7) $\varphi_j(E)$ is the wave function of the continous spectrum in the channel j, without resonance interference; $\varepsilon = (E - E\mu) / 1/2\ \Gamma_\mu^{tot}$ is the relative deviation from the resonance ; E_μ is the energy of the autoionising level μ ; q is the profile index of the resonance ; the sum of integrals in the denominator of (7) determines the total width of the autoionising level μ

$$\Gamma^{tot}_\mu = 2\pi \sum_j \left| \langle \phi_\mu | \hat{V} | \varphi_j(E) \rangle \right|^2 \quad (8)$$

3. Results and Discussion

Numerical calculations have been performed as follows. The excitation energies and wavefunctions of the autoionising levels were obtained as a result of diagonalisation of a 7×7 and a 12×12 matrix of electrostatic interaction in coulomb basis including the configurations 3lnl' with $l \leq 2$, $l' \leq 3$ and $3 \leq n \leq 5$. These basis are described by antisymmetrized products of the coulomb wavefunctions determined in the field of nuclear charge Z = 8.

The widths are calculated with the coulomb functions of the continuum spectrum with the charge Z = 8 for the electron wavefunction of the reduced ion and charge Z-1 for the photoelectron wavefunction.

In tables 1 and 2 we present the calculated excitation energies of the singlets autoionising states of the O^{6+} ion near the n = 3 threshold of the residual ion. Our results are given along with other theoretical results. The energies we have obtained are sufficiently stable to the dimension of the basis and are in good agreement with those of other authors [8-9].

The results of our work concerning the helium-like systems C^{4+} and N^{5+}[13] , and the results we obtained in the present work, show that the analysis of the structure of the wavefunctions of the autoionising states brings out an important mixing of configurations. In addition, by increasing the nuclear charge Z, the results show that it is no necessary to use a large basis of states for an accurate determination of the eigenvectors.

By using the assumption which consist of neglecting the direct coupling between the open channels, we have calculated the partial and total widths of the autoionising states of the helium-like oxygen ion O^{6+} . For total widths, the comparison of our results with those of other authors[8-9] in table 3, shows a good agreement . In the other hand, the partial widths corresponding to the decay of resonances through the four open channels 1SkP, 2SkP, 2PkS and 2PkD, reported in tables 4 and 5, show some differences with the results of Bachau et al [9]. We can notice that these differences depend on the considered autoionising state and concern particularly the partial widths corresponding to the transition to the continuum 1SkP. From table 4, one can see that the great differences between our results and those of Bachau et al [4] concern mainly the partial widths corresponding to the decay of autoionisation levels in which there is a D state, such as 3P3D, 3P4D and 4P3D. Regarding to the very weak probability for autoionisation transition to the ground state, these differences are probabily due to a problem of convergence depending of the size of the basis used in calculations. In addition, these differences could be explained by the sensitivity of the partial widths to the choice of the continuum wave functions.

We have also determine the relative decay of resonances to the fondamental state of the residual ion . From table 5, the analysis of the results shows that the probability for autoionisation transitions to excited states of ions is higher than that to the ground state. This result is in agreement with those obtained in the resonant photoionisation of helium-like systems with smaller Z [12, 14, 15]

4. Conclusion

Diagonalisation calculations used in the present paper allowed to obtain excitation energies and total widths in good agreement with those obtained by authors using other theoretical calculations. The results about partial widths calculated by neglecting the direct coupling between open channels , brings out some differences. Even though this approximation is quite reasonable for systems with a large nuclear charge Z [16], a detailed analysis of this problem requires a special attention.

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TABLE CAPTIONS

Table 1. Excitation energies (in a.u) of autoionisation states $^1P^{(e)}$ of the O^{6+} ion converging to the n = 3 threshold of residual ion

Table 2. Excitation energies(in a.u) of autoionisation states $^3P^{(e)}$ of the O^{6+} ion converging to the n = 3 threshold of residual ion

Table 3. Total widths (in eV)of autoionisation states $^1P^{(e)}$ of the O^{6+} ion converging to the n = 3 threshold of residual ion

Table 4. Partial widths (in eV) of autoionisation states $^1P^{(e)}$ of the O^{6+} ion near the n = 3 threshold of residual ion

Table 5. Partial widths Γ_j^{μ} (in eV) of autoionisation states $^1P^{(e)}$ and $^3P^{(e)}$ of the O^{6+} ; $\omega_\mu = \Gamma_1^\mu \left(\Gamma_1^\mu + \Gamma_2^\mu\right)^{-1}$ is the relative decay of the resonance to the n = 1 of O^{7+}

TABLE 1

States	PPF (a)	Feshbach formalism (b)	Present work
3S3P	6.628	6.624	6.622
3P3D	6.286	6.276	6.262
4S3P	5.297	5.296	5.312
4P3D	5.204	-	5.201
3P4D	5.199	-	5.174
3S4P	5.020	-	4.999
3D4F	4.986	-	4.916
5S3P	4.641	-	4.637
5P3D	4.596	-	4.571
3P5D	4.583	-	4.560
3S5P	-	-	4.407
3D5F	-	-	4.299

(a) Bachau et al[9]

(b) Bachau [8]

TABLE 2

States	PPF	Feshbach formalism	Present work
3S3P	6.714	6.712	6.711
3P3D	6.502	6.498	6.504
4S3P	5.262	5.261	5.294
4P3D	5.261	-	5.259
3P4D	5.139	-	5.202
4P3D	5.135	-	5.118
3D4F	5.031	-	5.082
3P5D	4.628	-	4.626
5S3P	4.618	-	4.589
3D5F	4.561	-	4.548
5P3D	-	-	4.517
3S5P	-	-	4.445

(a) Bachau et al [9]

(b) Bachau [8]

TABLE 3

States	Present work	PPF (a)	Feshbach formalism (b)
3S3P	0.46	0.40	0,44
3P3D	0.12	0.11	-
4S3P	0.0020	0.0019	-
4P3D	0.21	0.23	-
3P4D	0.045	0.044	-
3S4P	0.07	0.053	-
3D4F	0.0029	0.0022	-

(a) Bachau et al [9]

(b) Bachau[8]

TABLE 4

States	Transition channels			
	1SkP	2SkP	2PkS	2PkD
3S3P	0.003	0.41	0.0036	0.094
	(a) 0.0037	0.12	0.19	0.085
3P3D	$0.68 \cdot 10^{-5}$	0.020	0.017	0.047
	(a) $0.18 \cdot 10^{-2}$	0.0073	0.0019	0.096
4S3P	$0.15 \cdot 10^{-5}$	$0.76 \cdot 10^{-3}$	$0.82 \cdot 10^{-3}$	$0.43 \cdot 10^{-3}$
	(a) $0.20 \cdot 10^{-5}$	$0.70 \cdot 10^{-3}$	$0.81 \cdot 10^{-3}$	$0.36 \cdot 10^{-3}$
4P3D	$0.44 \cdot 10^{-4}$	0.08	0.023	0.047
	(a) $0.24 \cdot 10^{-2}$	0.069	0.12	0.042
3P4D	$0.34 \cdot 10^{-4}$	0.017	0.013	0.0099
	(a) $0.40 \cdot 10^{-3}$	0.016	0.018	0.0096
3S4P	0.0009	0.0015	0.0017	0.041
	(a) 0.0014	0.0029	0.0017	0.047
3D4F	$0.37 \cdot 10^{-6}$	$0.83 \cdot 10^{-3}$	$0.32 \cdot 10^{-5}$	0.0018
	(a) $0.19 \cdot 10^{-4}$	$0.28 \cdot 10^{-3}$	$0.36 \cdot 10^{-5}$	0.0019

(a) Bachau et al [9]

TABLE 5

Levels	Γ_j^μ , ω_μ	Present work	(a)
$^1P^{(-)}$ (1)	Γ_1^1	$0.38 \cdot 10^{-2}$	$0.37 \cdot 10^{-2}$
	Γ_2^1	0.46	0.405
	ω_1	$0.81 \cdot 10^{-2}$	-
$^1P^{(-)}$ (2)	Γ_1^2	$0.68 \cdot 10^{-5}$	$0.18 \cdot 10^{-2}$
	Γ_2^2	0.12	0.105
	ω_2	$0.56\ 10^{-3}$	-
$^1P^{(-)}$ (3)	Γ_1^3	$0.15 \cdot 10^{-5}$	$0.20 \cdot 10^{-5}$
	Γ_2^3	$0.20 \cdot 10^{-2}$	$0.19 \cdot 10^{-2}$
	ω_3	$0.75 \cdot 10^{-3}$	-
$^3P^{(-)}$ (1)	Γ_1^1	$0.57 \cdot 10^{-3}$	$0.19 \cdot 10^{-5}$
	Γ_2^1	0.11	0.105
	ω_1	$0.51 \cdot 10^{-2}$	-
$^3P^{(-)}$ (2)	Γ_1^2	$0.23 \cdot 10^{-5}$	$0.19 \cdot 10^{-5}$
	Γ_2^2	0.046	0.0427
	ω_2	$0.49 \cdot 10^{-4}$	-
$^3P^{(-)}$ (3)	Γ_1^3	$0.143 \cdot 10^{-3}$	$0.14 \cdot 10^{-4}$
	Γ_2^3	$0.73 \cdot 10^{-2}$	$0.73 \cdot 10^{-2}$
	ω_3	$0.195 \cdot 10^{-2}$	-

(a) Bachau et al [9]