Theoretical study on dielectronic recombination of O^{6+} ions in metastable states

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A computational scheme, based on the theory of the continuum-bound transitions of Bell and Seaton [J. Phys. B **18**, 1589 (1985)] and the close-coupling *R*-matrix approach, has been developed to treat dielectronic recombination (DR) in high-lying resonance-energy regions. This scheme and our presented numerical method to compute DR in low-lying resonance-energy regions [Phys. Rev. A **62**, 022706 (2000)] have been applied together to elucidate the experimental spectra of the DR of O^{6+} ions in the metastable $1s2s\ ^3S$ and $1s2s\ ^1S$ states. For comparison, a perturbative theoretical calculation of DR for O^{6+} has also been accompanied. The reasonable representation of the general dielectronic spectral shape is yielded by both our close-coupling and perturbative calculations. However, both the methods do not reproduce the experimental double-peak structure at $\sim 6-8$ eV. This shows that the further investigation on DR of this kind of ions is required both experimentally and theoretically.

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I. INTRODUCTION

Dielectronic recombination (DR) between free electrons and ions has attracted researchers' attention for many years owing to its importance in studies of astrophysics and plasma physics (see, e.g., [1,2]). Especially since the first direct measurements of DR were carried out [3–5], interest in DR has been heightened. A variety of theoretical approaches have been developed to investigate this process (see, e.g., [6–10]), and the resolution of experiments has been raised step by step [11–14]. So far a lot of progress has been made. The great enhancement of DR caused by external fields was found by LaGattuta and Hahn [15], Harmin [16], and Bartsch *et al.* [17]. Several groups showed that for heavy ions, relativistic and Breit corrections to the Auger rates lead to a drastic increase of the partial DR [18–20]. This increase may be conceived to be rational for high-Z and medium-Z ions. But recently it was found that the relativistic effect plays an important role for Li^+ ions with extremely low Z [21]. The occurrence of the experimental double-peak structure, which was not explained by LS-coupling *R*-matrix calculations, is attributed to fine-structure effects. In a theoretical research on photorecombination of highly charged few-electron uranium ions, Zimmermann, Grun, and Scheid [22] revealed that it is required to investigate higher-order QED effects beyond the Breit interaction in the electron-electron interaction due to its strong influence on the cross sections. The resonance-background interference in highly charged uranium ions was observed at the super-EBIT facility of the Lawrence Livermore National Laboratory [23]. Radiation damping was studied, and it turned out to be important [24–26]. A recent close-coupling calculation [27] for DR of C^{4+} removed the discrepancies between the experimental measurement and perturbative theoretical calculations [28,29].

Also there exist some experiments that are not interpretable by existing theory. The asymmetric Fano profiles for Ar-like Sc^{3+} and Ti^{4+}, due to the resonance-background interference, were predicted by the radiative optical-potential method [30], but the experimental search for such line shapes are in disagreement with the calculations within the experimental uncertainty [31]. In the merged-beam experiments and the ion-storage-ring experiments with several kinds of ions, the very strong increases of the measured radiation recombination rates in low relative-energy regions were seen over the calculated rates by several factors [32–34]. The temperature of these experimental electron beams is obtained by fitting dielectronic resonance peaks. The double-peak structures of several He-like ions, N^{5+}, O^{6+}, F^{7+}, and Si^{5+}, in the metastable states were not reproduced by perturbative calculations [11,35,36]. It was thought that this observation indicates a strong mixing of the three Rydberg series of resonances $1s2p(^1P)nl$, $1s2p(^3P)nl$, and $1s2s(^1S)nl$, and the multichannel-quantum-defect theory may be required to describe these systems [37].

All these issue a challenge to theoretical researchers and appeal exact treatments of photorecombination within nonperturbative theories. In a previous paper [26], based on the close-coupling *R*-matrix approach, we have presented a numerical method to calculate photorecombination in low-lying resonance-energy regions. However, this method is invalid when recombination into Rydberg series of resonances is invloved. In this investigation, based on the same *R*-matrix approach and Bell and Seaton's continuum-bound transition theory, we develop a computational scheme to treat DR in high-lying resonance-energy regions. This scheme and our presented numerical method to compute DR in the low-lying resonance-energy regions are applied together to elucidate the measured DR spectra of metastable O^{6+} ions in the heavy-ion storage-ring experiment [11,36]. A corresponding perturbative theoretical calculation is also made for comparison with that from the *R*-matrix approach.

In the second section, we will outline Bell and Seaton's theory [7] derived from the rigorous continuum-bound transition theory. In the third section, the results calculated are given and compared with the experiment of Andersen *et al.* [11]. The conclusions are summarized in the final section.

II. THEORY

The close-coupling *R*-matrix approach was presented by Burke, Hibbert, and Robb [38]. The details of this approach

can be found in Refs. [38,39] and therefore are not repeated in the present paper. Here we only describe Bell and Seaton's formalism [7]. This formalism was derived from the rigorous theory of continuum-bound transitions [40] to treat DR in the case of Rydberg series of resonances.

The process of emission of radiation in the optical continuum due to radiative capture of an electron by an ion was discussed by Davies and Seaton [40]. The general formulation including radiation damping was given. The scattering matrix $\mathcal{S}$ may be written with partitioning

$$\mathcal{S}=\begin{pmatrix} \mathcal{S}_{ee} & \mathcal{S}_{ep} \\ \mathcal{S}_{pe} & \mathcal{S}_{pp} \end{pmatrix}, \tag{1}$$

where $\mathcal{S}_{ee}$ represents the submatrix for electron-electron scattering allowing for radiative decays, $\mathcal{S}_{ep}$ represents that for photoionization, $\mathcal{S}_{pe}$ represents that for electron capture with the emission of a photon, and $\mathcal{S}_{pp}$ represents that for photon-photon scattering. $\mathcal{S}_{ee}$ and $\mathcal{S}_{pe}$ are written as, respectively,

$$\mathcal{S}_{ee}=\mathbf{S}[1-2\pi^2\mathbf{D}(1+\mathbf{Z})^{-1}\mathbf{D}^{\dagger}], \tag{2}$$

$$\mathcal{S}_{pe}=-2\pi i(1+\mathbf{Z})^{-1}\mathbf{D}^{\dagger}, \tag{3}$$

where **S** is the usual electron-electron scattering matrix in the absence of interaction with radiation fields, **D** is the reduced dipole matrix with its matrix element defined as

$$\mathbf{D}_{\gamma J,\gamma' J'}=\left(\frac{2\omega^3\alpha^3}{3\pi}\right)^{1/2}\frac{\langle \gamma J\|\mathbf{R}\|\gamma' J'\rangle}{(2J+1)^{1/2}}, \tag{4}$$

and

$$\mathbf{Z}(\Omega)=\pi^2\mathbf{D}^{\dagger}(\Omega)\mathbf{D}(\Omega)-i\pi\mathcal{P}\int dE\,\frac{\mathbf{D}^{\dagger}(E)\mathbf{D}(E)}{(E-\Omega)}. \tag{5}$$

In Eqs. (4) and (5), α is the fine-structure constant, ω is the photon energy in units of hartrees, $\mathbf{R}=\Sigma_i\mathbf{r}_i$ is the dipole operator, in which the summation is over all atomic electrons, γJ and $\gamma' J'$, respectively, specify the continuum and bound states of the atomic system, and $J(J')$ are the total angular momenta; the wave function of the continuum electron is normalized per unit hartree and $\mathcal{P}$ represents the Cauchy principal value of the integral.

From the above rigorous continuum-bound transition theory including radiation damping, and using the quantum-defeat theory, Bell and Seaton [7] construct a formalism in order to treat recombination in high-lying resonance-energy regions. The obtained electron-scattering matrix allowing for radiation damping is

$$\mathcal{S}_{ee}=\chi_{oo}-\chi_{oc}[\chi_{cc}-g(\nu)\exp(-2i\pi\nu)]^{-1}\chi_{co} \tag{6}$$

with

$$g(\nu)=\exp(\pi\nu^3A_r/z^2), \tag{7}$$

where ν is the effective quantum number, A_r is the radiative decay rate, z is the ion charge, $\chi_{\alpha\beta}$ denotes the submatrix for electron scattering from channel α to channel β, o represents the open channel, and c represents the closed channel. If we let $g(\nu)=1$ in Eq. (6), it means that the electron flux, which is tripped in the closed-channel resonances and decays radiatively to bound states of the $e+$ion system, is neglected. Namely, radiation damping is not taken into account.

For a given entrance channel α, the DR probability can be expressed in terms of $\mathcal{S}_{ee}$,

$$P_{\alpha}=(1-\mathcal{S}_{ee}^{\dagger}\mathcal{S}_{ee})_{\alpha\alpha}, \tag{8}$$

where the unitarity condition for the $\mathcal{S}$ matrix $\mathcal{S}_{ee}^{\dagger}\mathcal{S}_{ee}+\mathcal{S}_{pe}^{\dagger}\mathcal{S}_{pe}=1$ is used. Thus P_{α} can be obtained by the diagonal elements of the matrix

$$1-\mathcal{S}_{ee}^{\dagger}\mathcal{S}_{ee}=G(\nu)\chi_{oc}[\chi_{cc}-g(\nu)\exp(-2i\pi\nu)]^{-1}\times[\chi_{cc}^{*}-g(\nu)\exp(+2i\pi\nu)]^{-1}\chi_{co}^{*}, \tag{9}$$

where $G(\nu)=g(\nu)^2-1=\exp(2\pi\nu^3A_r/z^2)$. Using the representation in which $\overline{\chi}_{cc}$ is diagonal, the DR probability for the entrance channel α is rewritten [9],

$$P_{\alpha}=G(\nu)\sum_{\gamma}\left\{\left[\sum_{\gamma'}\overline{\chi}_{\alpha\gamma'}N_{\gamma\gamma'}\right]\times[\overline{\chi}_{\gamma\gamma}-g(\nu)\exp(-2i\pi\nu)]^{-1}\times[\overline{\chi}_{\gamma\gamma}^{*}-g(\nu)\exp(+2i\pi\nu)]^{-1}\left[\sum_{\gamma'}\overline{\chi}_{\gamma'\alpha}^{*}N_{\gamma\gamma'}^{*}\right]\right\}, \tag{10}$$

with

$$\overline{\chi}_{cc}=N^T\chi_{cc}N, \tag{11}$$

$$\overline{\chi}_{oc}=\chi_{oc}N, \tag{12}$$

$$\overline{\chi}_{co}=N^T\chi_{co}, \tag{13}$$

where the summations over $\gamma\gamma'$ run over all the closed channels contributing to DR, N is the diagonalizing matrix, and N^T is the transpose of N.

The total DR cross section is

$$\sigma(E)=\frac{\pi}{2k^2g}\sum_{\alpha}g_{\alpha}P_{\alpha}, \tag{14}$$

where k is the wave number of the incident electron, and g and g_{α} are the statistical weight of the recombining ion state and the continuum state, respectively.

To make a direct comparison with the experiment of Andersen *et al.* [11], we need to evaluate DR rate coefficients $\langle v\sigma\rangle$

$$\langle v\sigma\rangle=\int_0^{\infty}v\sigma f(v)d^3v, \tag{15}$$

where $f(v)$ is the experimental electron distribution, characterized by the pseudo-Maxwellian with the perpendicular temperature $T_\perp$ and the parallel temperature $T_\parallel$,

$$f(v)=\frac{m}{2\pi kT_\perp}\exp-mv_\perp^2/2kT_\perp\left[\frac{m}{2\pi kT_\parallel}\right]^{1/2}\times\exp[-m(v_\parallel-\Delta)^2/2kT_\parallel], \quad (16)$$

where m is the electron mass, k denotes Boltzmann's constant, $v_\perp$ and $v_\parallel$ are the electron-velocity components perpendicular and parallel to the ion-beam directions, respectively, and Δ is the detuning velocity that defines the relative energy ($\frac{1}{2}m\Delta^2=\varepsilon_r$).

III. RESULTS AND DISCUSSION

The formalism constructed by Bell and Seaton is a precise *ab initio* theory [7]. It reasonably includes radiation damping in electron-ion scattering by treating the outer electron as a *spectator*. This theory makes it practicable to exactly evaluate DR through an infinite series of resonances. From Sec. II, one may see that, in order to calculate the DR probability and cross section in high-lying resonance-energy regions using the formalism by Bell and Seaton, one first has to evaluate the open-closed (or closed-open) and closed-closed submatrices and the radiative decay rate of ion cores. We have written a code for this purpose on the basis of the close-coupling *R*-matrix approach [39]. The developed scheme was applied to the investigation of DR for O^{6+} ions in the metastable $1s2s\,^1S$ states. For the case of DR from the metastable $1s2s\,^3S$ states, our presented method in the previous paper [26] has been employed to perform the calculation. The investigation includes the determination of the target states and the calculation of recombination in the low- and high-lying resonance-energy regions. We adopted Hibbert's [41] CIV3 program to optimize the $2s$, $2p$, $3s$, $3p$, and $3d$ radial orbitals on the $2\,^{3,1}S$, $2\,^{3,1}P$, $3\,^{3,1}S$, $3\,^{3,1}P$, and $3\,^{3,1}D$ states, respectively. The $1s$ radial orbital was chosen to be the Hartree-Fock ground-state orbital of Clementi and Roetii [42]. The 11 lowest target states ($1\,^1S$, $2\,^3S$, $2\,^1S$, $2\,^3P$, $2\,^1P$, $3\,^3S$, $3\,^1S$, $3\,^3P$, $3\,^3D$, $3\,^1D$, $3\,^1P$) are included in our calculations.

For every symmetry of the total spin and orbital angular momentum and parity $SL\pi$, we carried out the *R*-matrix computations of DR from the $1s2s\,^1S$ state. The cross sections well converged are obtained when total orbital angular momentum $L=11$. This displays that the high partial waves have non-negligible contributions to the recombination from the $1s2s\,^1S$ state. To consider the effect of field ionization in the analyzing region of the experiment, the calculation was cut off after the maximum value of the effective principal quantum number $n_{max}=60$. The n_{max} was determined from the semiclassical field-ionization formula [36]. Figure 1 presents the DR rate coefficients $\langle v\sigma\rangle$ (solid curve) of O^{6+} in the metastable $1s2s\,^1S$ state. In the convolution to evaluate rate coefficients, the two temperatures $T_\perp=0.135$ eV and $T_\parallel=10^{-3}$ eV that describe the experimental electron distribution were employed. We also gave the $\langle v\sigma\rangle$ (dotted curve) from perturbation theory for comparison with the results from the close-coupling *R*-matrix approach. The perturbative theoretical method utilized in this paper can be found in Ref. [26], it therefore was omitted here. We use the single-configuration approximation to evaluate the cross sections in the transitions $1s2s\,^1S\varepsilon l_i\rightarrow 1s2p(^1P)nl\rightarrow 1s^2nl$ for the case of $n\leqslant 16$, and use the $1/n^3$ scaling law to obtain σ for the case of $16<n\leqslant n_{max}$. It may been seen that the difference between the DR cross sections from the *R*-matrix approach and those from the perturbation theory are not large. Also our perturbative results are quite in agreement with Badnell, Pindzola, and Griffin's [36] (their line is not plotted here). They have shown that the effects of configuration interaction are very small. It is surprising that the single-configuration approximation engenders such results.

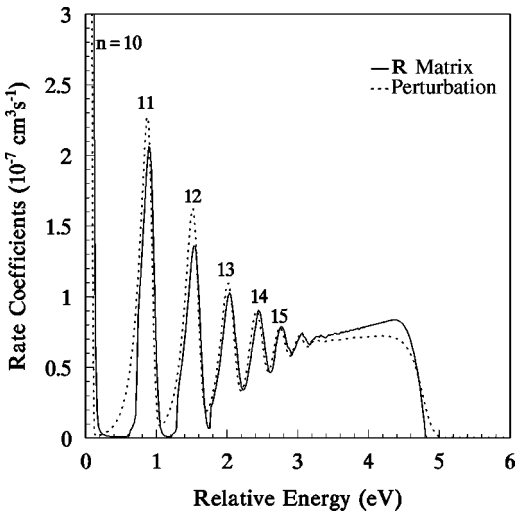

FIG. 1. Rate coefficients for dielectronic recombination of O^{6+} ions from the metastable $1s2s\,^1S$ state. The solid and dotted curve represents the results of the close-coupling *R*-matrix approach and perturbation theory, respectively.

Recombination from the $1s2s\,^3S$ was evaluated by using our presented numerical method [26]. This method is developed from the rigorous continuum-bound transition theory, and radiation damping is explicitly included by evaluating the Cauchy principal value of the integral in scattering matrices. In view of trivial contributions from the high partial waves to the DR cross sections, the states of the $e+O^{6+}$ system only with $L<5$ were retained in the present calculation. The rate coefficient calculated is depicted as a function of the relative energy ε_i in Fig. 2 (solid curve), and for comparison, the perturbative results are presented (dotted curve). It should be emphasized that the resonances from the perturbative calculation are shifted by -0.2 eV to match the experimental peaks. We noticed that the perturbation theory gives the comparable rate coefficients with the *R*-matrix method. Specially, the perturbative results are in good agreement with these in Ref. [36] (the curve is not accompanying here). From Fig. 2, one can see that above about 7.5 eV, dielectronic peaks drastically weaken. This is because the channels $1s2p(^3P)al$ and $1s2s(^1S)al$ are open above about 7.5 eV. It is these autoionization channels that attenuate dielectronic recombination. Badnell, Pindzola, and Griffin [36]

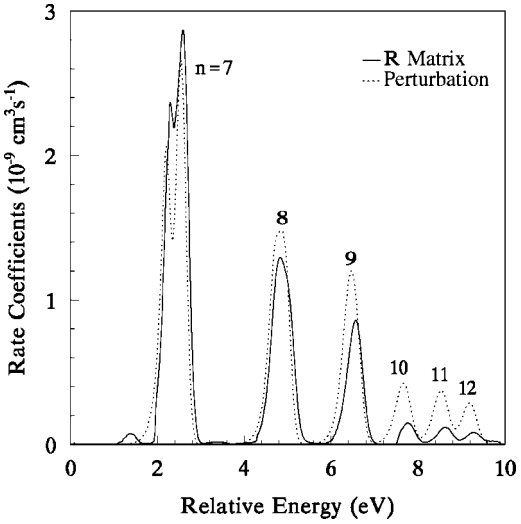

FIG. 2. The same as in Fig. 1, but for recombination from the $1s2s\,^3S$ state.

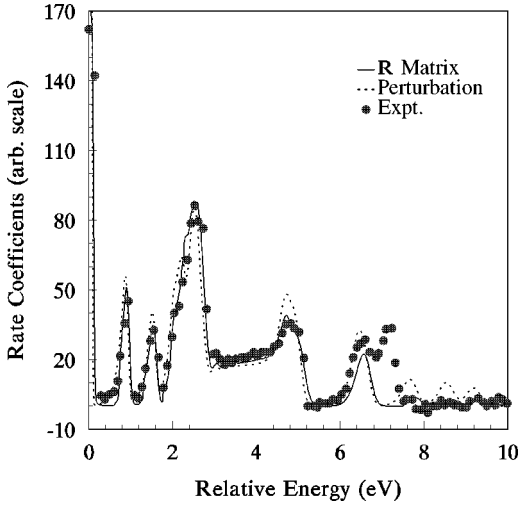

FIG. 3. Comparison between the theoretical and experimental (solid circles) rate coefficients for DR of O^{6+} ions in the mixed $1s2s\,^3S$ and $1s2s\,^1S$ states on an arbitrary scale. The ratio of the population fractions of the $1s2s\,^3S$ and $1s2s\,^1S$ is set to be 105 for the *R*-matrix calculations and 110 for the perturbative calculations.

studied the degree to which these channels affect DR in the metastable $1s2s\,^3S$ state by including and excluding transitions to $1s2p\,^3P$ and $1s2s\,^1S$ continua. A marked effect was displayed [36]. In Fig. 2 the higher perturbative values after $\sim$7.5 eV (dotted curve) may be due to the computational errors of the widths of autoionization from these resonances to the $1s2p\,^3P$ and $1s2s\,^1S$ states.

The exact population fractions of the target ion O^{6+} in the ground and metastable $1s2s\,^1S$ and $1s2s\,^3S$ states in the experiments of Andersen *et al.* [11,12] are unclear. The state population was roughly estimated to be 70% for $1s^2$, 30% for $1s2s\,^1S$, and $\leqslant$1% for $1s2s\,^3S$ [12]. From the rough estimate, the ratio of the population fractions of the ions in the first two states may be 30–300 (whereas 1–0.1 % for $1s2s\,^3S$). Since the recombination is only from the $1s2s\,^1S$ and $1s2s\,^3S$ states in the energy region concerned (0–14 eV), the calculated rate coefficients should be multiplied by the ratio to make a comparison with the observation. We adjusted the ratio until the best agreement between theory and experiment was reached. Figure 3 presents the DR rate coefficients evaluated from the *R*-matrix approach (solid curve) and from the perturbation theory (dotted curve) along with the experimental measurement of Andersen *et al.* [11]. In Fig. 3 the suitable ratios for the $1s2s\,^3S$ and $1s2s\,^1S$ are 105 for the *R*-matrix calculations and 110 for the perturbative ones. From this figure it may be found that the reasonable representation of the general dielectronic spectral shape is yielded, but both our close-coupling and perturbative calculations do not reproduce the experimental double-peak structure at $\sim$6–8 eV.

This discrepancy may not be due to the treatment of radiation damping, as the present computation pretty reliably includes damping effects. We do not think that the difference may be attributed to the treatment of electron correlation. This is because the solid curve evaluated on the basis of the close-coupling *R*-matrix approach is the multichannel result; the electron correlation of the $e+$ion system is well involved. Also the treatment of the resonance-resonance (RR) interference and resonance-background (RB) interference may not result in the discrepancy, since our method [26] is suitable for systems with stronger RR and RB interference. However, we noticed that this result was obtained in the *LS*-coupling approximation. We must check the relativistic effect in the recombination. The study showed that the effect plays an important role in DR for He-like lithium with extremely low Z [21]. The occurrence of an experimental double peak is surprisingly attributed to relativistic corrections. We found that whether a resonance is significant depends not only on the Auger (Γ_a) and radiative widths (Γ_r) of the resonance themselves but also on the Γ_a and Γ_r of the dominant resonances. In the $e+O^{6+}$ system, the Γ_a of the resonances due to the spin-orbital interaction at $\sim$6–8 eV are by far narrower than the Γ_a of the dominant resonances, but the Γ_r, which are decided by the transitions from the inner-shell electrons, of all the resonances at the experimental-energy regions concerned are almost the constants which are much larger than the Γ_a due to the spin-orbit interaction. In this system, therefore, it is impossible to attribute the double-peak structure to the relativistic effect. There was the same discrepancy between the experiment and the perturbative calculation in Ref. [36]. However, it should be mentioned that Badnell, Pindzola, and Griffin [36] performed a simplified-model calculation to investigate effects of mixing of the resonance through interaction with the adjacent continua on DR cross sections. They assume that the resonances $1s2s(^1S)nl$ and $1s2p(^3P)nl$ ($n\geqslant 20$) interact with the resonances $1s2p(^1P)9l$ through the adjacent continua to acquire radiative strength from the $1s2p\,^1P \rightarrow 1s^2\,^1S$ channel, and thus DR cross sections through the intermediate states $1s2s(^1S)nl$ and $1s2p(^3P)nl$ may be enhanced compared with the DR cross sections without such interactions. Namely, a double-peak structure may appear owing to the interactions. Their model evaluation displayed such a structure. Meanwhile, in Ref. [36] a close-coupling

investigation was appealed to prove that this experimental feature might be explained in this way. But neither Price's [43] nor our close-coupling *R*-matrix calculations (see Fig. 3) give rise to the similar result. Because the mixing effect through the continua are incorporated into our calculations, obviously it is not possible for this experimental feature at $\sim 6-8$ eV to be explained in this way. The discrepancy between the experiment and all the theoretical computations except for the simplified-model calculation is not explained. This displays that further experimental and theoretical work are necessary to understand deeply dielectronic recombination for O^{6+}. For example, it may be valuable to measure DR from the single, not mixed, metastable state and to see the difference between experiment and theory. Because of the development of the experimental technique, to do so at present is possible (see, e.g., [44]).

IV. CONCLUSIONS

We have developed a computational scheme to calculate dielectronic recombination in high-lying resonance-energy regions. Since this scheme is based on Bell and Seaton's continuum-bound transition theory [7] and the close-coupling *R*-matrix approach, radiation damping in electron-ion scattering and electron-electron correlation are effectively involved. This scheme and our presented numerical method [26] have been applied together to the investigation of dielectronic recombination of O^{6+} ions in the metastable states. For comparison, the calculations from perturbation theory are also accompanied. Although the reasonable representation of the general experimental dielectronic spectral shape is yielded by both our close-coupling and perturbative calculations, both the methods do not reproduce the double-peak structure of the experiment of Andersen *et al.* [11] at the $\sim 6-8$ eV energy region. This discrepancy remains to be explained. Our study shows that further theoretical and experimental work may be required.

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