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Measure for the effect of quantum interference between radiative and dielectronic recombination

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The electron-ion photorecombination (PR) cross section is known to have an asymmetric energy profile, as a result of quantum interference between direct radiative and dielectronic recombination. We introduce a parameter that reflects the degree of this asymmetry and use it to identify PR transitions for which the effects of interference may be observable. Significantly asymmetric PR cross-section profiles are found for a few PR transitions from He-like Ar and Fe via $1s2l2l'$ autoionizing levels. The profile asymmetry parameter provides a physical measure for the scaling of the interference effect with the ion charge.

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The photorecombination (PR) process of a multiply charged ion with a free electron, involving radiative emission, can have a significant influence on the atomic-state kinetics and electromagnetic spectra in electron-ion beam interactions and in laboratory and astrophysical plasmas. The PR process has been traditionally described in terms of two distinct recombination mechanisms. The first is nonresonant or direct radiative recombination (RR), which is the inverse of the ordinary photoionization process. The second corresponds to the next diagrammatic order and is the two-step, resonant process, known as dielectronic recombination (DR). These two recombination mechanisms are usually treated as independent, noninterfering processes. It has been recognized, however, that this traditional description is not strictly permissible within the framework of a rigorous quantum-mechanical theory [1–4]. At low densities, for which collisional dephasing and relaxation phenomena can be ignored, RR and DR must be treated as coherent, interfering components of a single electromagnetic process occurring between the relevant initial and final atomic states. Several investigations have been carried out in the search for prominent signatures of the quantum-mechanical interference between RR and DR (e.g., Refs. [5–7]). The most conspicuous manifestation of this interference is expected to be the asymmetric energy profile of the total PR cross section. This asymmetric profile has been observed by Knapp *et al.* [8] for the PR of very highly ionized uranium in an electron-beam ion trap (EBIT) experiment.

In the present work, we introduce a parameter that reflects the degree of asymmetry in the total PR cross section and use it to identify PR transitions exhibiting a prominent asymmetry. The projection-operator and resolvent-operator approach of Jacobs, Haan, and Cooper [2,3,9] is employed in the lowest order of perturbation theory to calculate the profile asymmetry parameter, as well as the cross sections for PR of He-like Ar ($Z=18$) and Fe ($Z=26$) through the $1s2l2l'$ autoionizing levels. The relativistic multiconfiguration Hebrew University Lawrence Livermore atomic code (HULLAC) package developed by Bar-Shalom *et al.* [10] is adapted to provide the partial-wave radiative emission and autoionization amplitudes, including the required phases.

It has been shown [3] that the total cross section for photorecombination from the initial level i of the recombining ion to the final level f of the recombined ion, near the energy of a discrete doubly excited autoionizing level d, can be expressed as a sum of three contributions: the RR cross section, the DR cross section, and the term representing the interference (denoted by int) between the RR and the DR transition amplitudes:

$$\sigma_{if}^{\mathrm{PR}}(\varepsilon)=\sigma_{if}^{\mathrm{RR}}(\varepsilon)+\sigma_{idf}^{\mathrm{DR}}(\varepsilon)+\sigma_{idf}^{\mathrm{int}}(\varepsilon). \tag{1}$$

ε denotes the kinetic energy of the incident free (beam or plasma) electron.

In the lowest nonvanishing order of perturbation theory, the interference contribution can be expressed in terms of the familiar autoionization rate A_{di}^{a} and DR cross section:

$$\sigma_{idf}^{\mathrm{int}}(\varepsilon)=\sigma_{idf}^{\mathrm{DR}}(\varepsilon)\,\frac{4(E_i+\varepsilon-E_d)}{\hbar A_{di}^{a}}\,\frac{1}{Q_{idf}}. \tag{2}$$

E_i and E_d represent the energies of the atomic levels i and d, respectively. Equation (2) can be obtained from the more

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general nonperturbative expression presented in Eq. (86) of Ref. [3], by taking the continuum-continuum coupling factor [3] to be unity and by assuming that $1/(Q_{idf})^2$ vanishes. The Fano parameter Q_{idf} can be defined in terms of the standard reduced partial-wave matrix elements for RR from level *i* to level *f* and for autoionization from level *d* to level *i*, as well as by the reduced matrix element for the radiative transition from level *d* to level *f*:

$$\frac{1}{Q_{idf}}=\frac{\pi}{(2J_d+1)^{1/2}}\frac{\sum_{\kappa}\langle fJ_f\|H_{\rm em}\|iJ_i,\varepsilon\kappa;J_d\rangle\langle iJ_i,\varepsilon\kappa;J_d\|H_{\rm es}\|dJ_d\rangle}{\langle fJ_f\|H_{\rm em}\|dJ_d\rangle}. \quad (3)$$

$H_{\rm em}$ is the Hamiltonian for the electromagnetic interaction, which is responsible for RR as well as for stabilizing radiative emission. The electric-dipole approximation has been adopted in the present computations. $H_{\rm es}$ represents the Hamiltonian for the electrostatic electron-electron interaction, which is responsible for autoionization. J_i, J_d, and J_f are the total angular-momentum quantum numbers of the atomic levels *i*, *d*, and *f*, respectively. The quantum number κ represents both the orbital and total angular-momentum quantum numbers of the free electron.

The total PR cross section in Eq. (1), including the interference contribution, can be rewritten in the familiar Fano-profile form [11] by generalizing the Fano parameters to include radiative coupling (Sec. IV of Ref. [12]). The energy (ε) dependence of the PR cross section, thus, corresponds to a radiatively modified Fano-type asymmetric energy-profile function. It is advantageous to define a measure for the importance of the interference effect. Badnell and Pindzola [5] used the difference between energy-averaged cross sections calculated with and without the inclusion of the interference contribution. This procedure can give an estimation of the interference contribution to the energy-integrated PR rates, but cannot describe the energy-dependent asymmetry in the PR cross-section profile.

We propose an alternative, more sensitive method for describing the degree of asymmetric behavior characteristic of the interference between RR and DR. In this method, we evaluate the DR and interference contributions at the two energies,

$$\varepsilon_{\pm 1/2}=E_d-E_i\pm\frac{\Gamma(d)}{2} \quad (4)$$

for which the interference contribution, due to a single (isolated) resonance *d*, has an extremum [maximum or minimum, depending on the sign in front of $\Gamma(d)$] and the Lorentzian function describing the energy dependence of the (unperturbed) DR cross section attains one-half of its maximum value. $\Gamma(d)$ is the total width of the doubly excited level *d* due to the radiative emission and autoionization processes:

$$\Gamma(d)=\hbar\left(\sum_f A_{df}+\sum_i A^a_{di}\right). \quad (5)$$

A_{df} is the usual Einstein coefficient for the radiative transition from level *d* to level *f*. Using Eq. (2), the absolute value of the ratio of the interference contribution and the DR cross section, evaluated at $\varepsilon_{\pm 1/2}$, can be expressed in the form

$$R^{\rm int}=\left|\frac{\sigma^{\rm int}_{idf}(\varepsilon_{\pm 1/2})}{\sigma^{\rm DR}_{idf}(\varepsilon_{\pm 1/2})}\right|=\frac{2\Gamma(d)}{\hbar A^a_{di}}\left|\frac{1}{Q_{idf}}\right|. \quad (6)$$

The profile asymmetry parameter $R^{\rm int}$ provides a sensitive measure for the degree of asymmetry in the PR cross-section profile. A larger value of this parameter corresponds to a more asymmetric profile. Note that $R^{\rm int}$ in Eq. (6) is proportional to $1/Q_{idf}$, but gives a more direct characterization of the degree of asymmetry than $1/Q_{idf}$. This should also be contrasted with the $1/(Q_{idf})^2$ dependence of the energy-averaged interference contribution given by Eq. (13) in Ref. [5]. The profile asymmetry parameter $R^{\rm int}$ is half the reciprocal of the lowest-order line-shape parameter $\hat{q}$ defined by Haan [12], which was shown to be equivalent to the generalized *Q* value given by Bell and Seaton [13].

We report the results of detailed level-specific computations for the PR cross section of He-like Ar and Fe in the $1s^2$ ground state (*i*), in the energy region of the (Li-like) $1s2l2l'$ autoionizing levels (*d*). The calculated values of $R^{\rm int}$ are given in Table I. Each level-specific ($i\rightarrow d\rightarrow f$) DR transition is labeled following the notational convention of Gabriel [14]. It can be seen that most of the PR transitions have $R^{\rm int}$ values less than 0.1, which indicates that experimental detection of the interference effect for these transitions would be difficult. For the PR transition denoted by *i* from He-like Ar, $R^{\rm int}$ has an unusually high value of 0.551. Accordingly, this transition may represent the best candidate for experimental detection of the asymmetric profile among these PR transitions from He-like Ar. For He-like Fe, we identify four DR transitions with the property $R^{\rm int}>0.1$. This suggests that highly charged ions could offer more promising candidates for observation of prominent asymmetric cross-section profiles. The detailed dependence of the interference effect on the ion charge is investigated elsewhere [15].

Figure 1 depicts the small portion of the He-like Ar level-specific PR cross section as a function of the incident electron energy in the vicinity of the *l* resonance transition. Our

TABLE I. The parameter R^{int} [Eq. (6)], which reflects the degree of asymmetry in the total PR cross section profile due to interference between RR and DR, evaluated for recombination of He-like Ar^{16+} and Fe^{24+} through the Li-like autoionizing levels $1s2l2l'$. The resonance transitions are labeled in accordance with the notation of Gabriel [14]. The most asymmetric transition for each ion is indicated in boldface. Numbers in square brackets represent powers of 10.

Transition label [Ref. [14]]	R^{int} Ar^{16+}	R^{int} Fe^{24+}
a	5.61[−3]	8.86[−3]
b	4.62[−2]	1.49[−1]
c	9.14[−2]	1.33[−1]
d	3.99[−2]	4.81[−2]
e	7.64[−3]	9.68[−3]
f	2.65[−3]	5.18[−3]
g	5.14[−2]	9.69[−2]
h	3.87[−2]	1.93[−1]
i	5.84[−3]	1.40[−2]
j	7.46[−3]	9.71[−3]
k	6.64[−3]	1.04[−2]
l	**5.51[−1]**	1.45[−2]
m	3.65[−3]	8.16[−3]
n	5.39[−3]	2.72[−2]
o	1.12[−2]	1.06[−2]
p	9.82[−3]	7.33[−3]
q	2.36[−2]	**2.09[−1]**
r	1.21[−2]	2.00[−2]
s	1.90[−2]	3.23[−2]
t	1.16[−2]	1.48[−2]
u	1.20[−2]	3.11[−2]
v	1.01[−2]	3.38[−2]

calculations indicate that significant interference effects may be observable for this transition. The three partial contributions [Eq. (1)] are illustrated in Fig. 1 by means of separate curves. It can be seen that, for this relatively weak DR transition, the interference contribution produces a substantial asymmetric PR cross-section profile. It should be noted that, in the total PR cross section as a function of the incident electron energy, the existence of two alternative radiative-decay channels gives rise to overlapping resonance profiles. Consequently, the asymmetric profile associated with the *l* resonance alone, which is plotted in Fig. 1, can be observed only by the detection of the distinct x-ray photons emitted in the radiative decays to different levels *f* [16,17]. Moreover, the observation of the very narrow (sub-eV) width of the *l* resonant-transition profile may be difficult with the energy resolution of present electron-beam experiments. In the He-like Fe PR cross section, the *q* resonance channel is found to exhibit the most asymmetric cross-section profile. Similar to the case of the *l* transition for Ar, the *q* feature for Fe is predicted to be relatively weak in comparison with the more prominent $1s2l2l'$ features in the Fe group. The calculated profile asymmetry parameter describing this resonance channel is not as large as that for the *l* resonance in Ar. In contrast

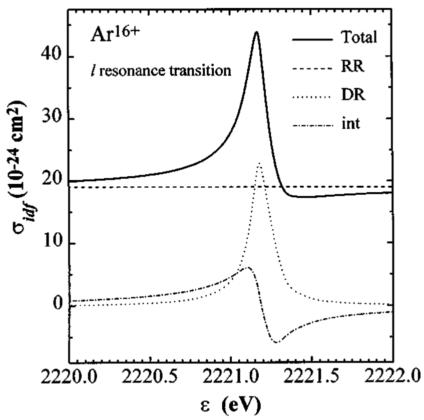

FIG. 1. The cross section for PR of He-like Ar^{16+} in the vicinity of the level-specific resonance channel *l*. The total PR cross section (σ^{PR}) is represented by a solid line. The direct nonresonant RR cross section (σ^{RR}) is indicated by a dashed line, the two-step, resonant DR cross section (σ^{DR}) is indicated by a dotted line, and the interference contribution (σ^{int}) is indicated by a dash-dotted line.

with the *l* resonance feature, however, the *q* feature is relatively isolated in the electron-energy spectrum.

In conclusion, we have introduced a parameter for the degree of asymmetry in the total electron-ion photorecombination cross-section profile. This parameter is computed for the recombination of He-like Ar and Fe via the $1s2l2l'$ autoionizing levels and used to analyze the influence of the interference between RR and DR on the total PR cross section. For certain relatively weak transitions, significant effects of quantum-mechanical interference are revealed in the form of radiatively modified, asymmetric (Fano-type) cross-section profiles. It is found that, in many cases, the asymmetric profile will be observable only with the detection of the individual photons emitted in the alternative radiative-decay channels of the recombination process. Because of the sub-eV width of the DR resonance features, the observation of the detailed energy profile may be difficult with the resolution in current electron-ion–beam experiments. The profile asymmetry parameter enables a systematic and detailed investigation of the interference between RR and DR, including the dependence on the ion charge *z* and on the principal quantum number *n* of the outer electron in the autoionizing state. This analysis shows that asymmetric profiles can be especially significant for both high-*z* and for low-*z* ions as well as for high-*n* and low-*n* levels, but less so for the intermediate cases [15]. Furthermore, by using a density-matrix approach, a generalized unified theory [18] will be applied to treat, on an equal footing and in a self-consistent manner, the interference between RR and DR together with collisional and radiative relaxation processes. In a further extension of this investigation, it will be necessary to consider the influence of electric and magnetic fields.

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