Effects of radiative decay on the bound-continuum transition of highly charged atomic ions

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In a system consisting of an electron and a highly charged ion, interaction with the radiation field is strong, and radiation-damping effects must be accurately taken into account. The present work provides a numerical method to study the radiation-damping effect in the processes of photoionization, radiative recombination, and electron scattering. A simple calculation is made for Fe^{24+}, $Xe^{52+}(1s2s)+h\nu \leftrightarrow Fe^{25+}$, $Xe^{53+}(1s)+e$. Special emphasis is placed on the nonapplicability of conventional first-order perturbation theory to photoinduced autoionization of a highly charged ion. The interference effect between the resonant and the nonresonant parts is found to be negligible in the present cases.

I. INTRODUCTION

Photoionization cross sections of atoms are usually calculated by using an equation

$$Q_{\mathrm{PI}}=C|(f|\,\mathbf{A}\cdot\mathbf{P}|i)|^2\ ,$$

where C is some factor, $H_{\mathrm{rad}}=\mathbf{A}\cdot\mathbf{P}$ is the interaction with the radiation field, $\mathbf{A}$ is the vector potential, $\mathbf{P}$ is the momentum of the atomic electrons, and f and i indicate a final continuum and an initial bound state, respectively. In many cases, it is believed that this conventional equation is accurate without any doubt. It should be noted, however, that the conventional equation is based on first-order perturbation theory because only the first-order effect of H_{rad} is retained. The interaction with the radiation field becomes very strong for a highly charged ion. In that case, the higher-order effects of H_{rad} would not be negligible. Suppose that a bound electron is excited to a continuum state by absorbing a photon. This is caused by the action of the first order in H_{rad}. However, if we consider the higher-order effect in H_{rad}, the excited electron can simultaneously emit a photon to fall again in a bound state. This kind of phenomenon is called a radiation-damping effect.[1,2] The radiation-damping effect is well known as a cause of bound-state natural width. In this study, we consider its effect on bound-continuum transitions.

The breakdown of first-order perturbation theory has already been pointed out in the study of dielectronic recombination.[1] A resonance state, formed during the collision between an electron and a positive ion, has two decaying branches, namely, autoionization and radiative emission. Let Γ_a be the probability for autoionization and Γ_r the probability for radiative emission. The importance of the radiative effect depends on the ratio Γ_r/Γ_a. Only if this ratio is much less than unity can first-order perturbation theory be applied to dielectronic recombination.[1] Since Γ_r/Γ_a is roughly proportional to the fourth power of the ion charge, it can be greater than unity for highly charged ions.

In order to treat accurately the radiative effect in electron scattering by ions, Davies and Seaton[2] applied the Wigner-Weisskopf theory of radiation damping. They obtained a general formula for the S matrix including a radiative channel. Once this S matrix has been calculated, one can directly obtain the cross sections for photoionization, radiative recombination, and also for electron scattering by ions in which the radiation field is coupled.

However, it is not easy to calculate the S matrix without making any approximation. Recently, Bell and Seaton[3] showed that, when a quantum-defect theory[4] is applicable, the S matrix can be reduced to a very simple form. This enables one to calculate the S matrix for processes related to high-lying resonances in a Rydberg series. The quantum-defect theory is not valid for describing low-lying resonances. There have been many published calculations of cross sections or rate coefficients for dielectronic recombination. For low-lying resonances, however, all these calculations introduce some approximations: (i) the wave function of the resonance states is calculated by use of a computer code for bound states; (ii) the probabilities Γ_a and Γ_r are calculated within a distorted-wave-type method;[5–7] (iii) no consideration is taken into account of the nonresonant contribution (direct radiative recombination), and its interference effect with the resonant contribution is consequently neglected.

In the present report, we develop a numerical method to calculate the S matrix, including the radiative channels in the energy range relating to the low-lying resonances. We use the R-matrix method to obtain accurate values of the collisional S matrix and the dipole matrix. This method is the basis for a calculation free of the approximations mentioned above. We also discuss the radiation-damping effect on the process of photoionization.

II. THEORY

We partition the S matrix including radiation channels into

$$\underline{S}=\begin{bmatrix}\underline{S}_{e\text{-}e} & \underline{S}_{e\text{-}p}\\ \underline{S}p\text{-}e & \underline{S}_{p\text{-}p}\end{bmatrix}, \tag{1}$$

where e-e means the submatrix for electron-electron scattering, e-p, for photoionization, p-e for radiative recombination, and p-p for photon-photon scattering. By solving the radiation-damping equation for bound-continuum transitions, Davies and Seaton gave[2]

$$\underline{S}_{e\text{-}e}=\underline{S}_{\text{scatt}}[1-2\pi^2\underline{D}(1+\underline{L})^{-1}\underline{D}^{\dagger}], \tag{2}$$

$$\underline{S}_{p\text{-}e}=-2\pi i(1+\underline{L})^{-1}\underline{D}^{\dagger}, \tag{3}$$

where $\underline{S}_{\text{scatt}}$ is the usual S matrix including no radiative coupling, and $\underline{D}$ is the reduced dipole matrix in the form

$$D_{J\gamma,J'\gamma'}(E)=\left[\frac{2\omega^3\alpha^3}{3\pi}\right]^{1/2}\frac{(EJ\gamma||\sum_i r^{(i)}||J'\gamma')}{(2J+1)^{1/2}}, \tag{4}$$

and

$$\underline{L}(E)=-i\pi\int dE'\frac{\underline{D}^{\dagger}(E')\underline{D}(E')}{E'-E-i\epsilon}. \tag{5}$$

In this study, we consider only the dipole term as the interaction with the radiation field. In Eq. (4), the continuum and the bound states are specified by $(EJ\gamma)$ and $(J'\gamma')$, respectively, (J and J' being the total angular momenta); the summation of the dipole operator is taken over all the electrons; E and ω are the total and the photon energies, respectively (i.e., $E=E_{\gamma'J'}+\omega$); and α is the fine-structure constant. The wave function of the continuum state is normalized to unit energy with the usual scattering (S matrix) boundary condition. We can show in a way similar to the one followed by Davies and Seaton[2] that $\underline{S}_{e\text{-}p}$ and $\underline{S}_{p\text{-}p}$ are given by

$$\underline{S}_{e\text{-}p}=-2\pi i\underline{D}^{*}(1+\underline{L}^{t})^{-1}, \tag{6}$$

$$\underline{S}_{p\text{-}p}=2(1+\underline{L}^{t})^{-1}-1. \tag{7}$$

The dipole matrix element (4) scales as z^2, where z is the ion charge.[6] Hence for a highly charged ion, the dipole matrix element becomes very large. This is the reason why first-order perturbation theory fails for highly charged ions. Because of the inverse matrix $(1+\underline{L})^{-1}$ or $(1+\underline{L}^{t})^{-1}$ appearing in Eqs. (2), (3), (6), and (7), the S matrix itself does not take a large value. It is easily shown that the S matrix satisfies unitarity.[2,3] From Eqs. (2), (3), (6), and (7), one can obtain accurate cross sections for the corresponding processes.

If we retain only the first-order term of $\underline{D}$, we have

$$\underline{S}^{(1)}_{e\text{-}e}=\underline{S}_{\text{scatt}}, \tag{8}$$

$$\underline{S}^{(1)}_{p\text{-}e}=-2\pi i\underline{D}^{\dagger}, \tag{9}$$

$$\underline{S}^{(1)}_{e\text{-}p}=-2\pi i\underline{D}^{*}, \tag{10}$$

$$\underline{S}^{(1)}_{p\text{-}p}=1. \tag{11}$$

Equation (10) gives the conventional first-order perturbation formula for photoionization. Photon-photon scattering is a higher-order effect of $\underline{D}$ because the approximated S matrix (11) is unity.

The complex conjugate of Eq. (4) $\underline{D}^{*}$ is just equal to the dipole matrix (except for a state-density factor) appearing in the conventional calculation of photoionization [see also Eq. (10)] and can be calculated in the usual way. However we need to evaluate the integral (5). The dipole matrix generally has poles, which originate from the continuum wave function and give the resonant contribution. Since the pole positions determine the integral value, it is very important to know the analytical properties of the continuum wave function. A detailed study of these properties have been given by Seaton.[8] According to his conclusion, we can write the dipole matrix element in the simple form

$$D_{J\gamma,J'\gamma'}(E)=D^{0}_{J\gamma,J'\gamma'}(E)+\sum_{\lambda}\frac{A^{\lambda}_{J\gamma,J'\gamma'}}{E-(Z^{\lambda})^{*}}, \tag{12}$$

where the first and the second terms on the right-hand side correspond to the nonresonant and the resonant contributions, respectively. The complex energy Z^{λ} is given by

$$Z^{\lambda}=E^{\lambda}_{a}-\frac{i}{2}\Gamma^{\lambda}_{a}, \tag{13}$$

which is the definition of a resonance λ position E^{λ}_{a} and width Γ^{λ}_{a}.

The form (12) allows some overlapping of resonances. However, when the resonances overlap strongly with each other, the dipole matrix element may not be expressible in the form (12). In the present study, we are concerned with nonoverlapping resonances and energy regions close to resonances. Hence we may assume that D^0 is a slowly varying function of the energy, and that A^{λ} and Z^{λ} are independent of energy. We fit the dipole matrix numerically to the form (12). Substituting the result into the integral (5) and evaluating it by contour integration, we finally obtain

$$\begin{aligned}L_{J'\gamma'J''\gamma''}(E)=&\pi^2\sum_{J,\gamma}[D^{0}_{J\gamma,J'\gamma'}(E)]^{*}D^{0}_{J\gamma,J''\gamma''}(E)\\&+2\pi^2\sum_{J,\gamma,\lambda}\frac{(A^{\lambda}_{J\gamma,J'\gamma'})^{*}D^{0}_{J\gamma,J''\gamma''}(E)}{E-Z^{\lambda}}\\&+2\pi^2\sum_{J,\gamma,\lambda,\lambda'}\frac{(A^{\lambda}_{J\gamma,J'\gamma'})^{*}A^{\lambda'}_{J\gamma,J''\gamma''}}{(E-Z^{\lambda})[Z^{\lambda}-(Z^{\lambda'})^{*}]}.\end{aligned} \tag{14}$$

III. CALCULATIONS

We performed a simple calculation for the following process:

$$A^{Z+}(1s)+e\leftrightarrow A^{(Z-1)+}(2s2p)\leftrightarrow A^{(Z-1)+}(1s2s)+h\nu, \tag{15}$$

where we considered both Fe^{25+} and Xe^{53+} for A^{Z+}. The continuum ($1sE$) and the bound ($1s2s$) states have symmetry $^1P^0$ and $^1S^e$, respectively (LS coupling is as-

sumed for addition of the angular momentum and relativistic effects are neglected). We have used the R-matrix computer code[9] to calculate the dipole matrix element. The $1s$, $2s$, and $2p$ states of the hydrogenic target ion are coupled in the calculation. Twenty continuum orbitals have been included in the R-matrix expansion of the total wave function.

The $2s2p$ resonance is well isolated. Hence the dipole matrix element can be accurately approximated by

$$D(E)=D^0(E)+\frac{A}{E-Z^*} , \tag{16}$$

where D^0 and A are constant in energy [subscripts have been omitted in Eq. (16) for simplicity]. In this case, Eq. (14) becomes

$$L(E)=\pi^2|D^0(E)|^2+2\pi^2\frac{A^*D^0(E)}{E-Z}+2\pi^2\frac{|A|^2}{(E-Z)(Z-Z^*)} . \tag{17}$$

The probability for the electron-photon or photon-electron process is given by

$$P_{e\text{-}p}=P_{p\text{-}e}=|S_{e\text{-}p}|^2=\frac{4\pi^2|D|^2}{|1+L|^2} . \tag{18}$$

From the unitarity of the S matrix, the quantities $P_{e\text{-}p}$ and $P_{p\text{-}e}$ cannot exceed unity. The partial cross sections for photoionization ($Q_{\rm PI}$) and radiative recombination ($Q_{\rm RR}$) are, respectively,

$$Q_{\rm PI}=\frac{\pi}{2\alpha^2\omega^2}\frac{2J+1}{2J'+1}P_{e\text{-}p} , \tag{19}$$

$$Q_{\rm RR}=\frac{\pi}{2k^2g}(2J+1)P_{p\text{-}e} , \tag{20}$$

where k is the wave number of the incident electron, and g is the statistical weight factor of the recombining ion (A^{Z+}) state.

We obtain the resonance position (13) by fitting the K-matrix elements using the code of Bartschat and Burke.[10] In the present cases, we obtained $E_a=347.794\,97$ Ry and $\Gamma_a=0.008\,830\,6$ Ry for $e+Fe^{25+}$, and $E_a=1478.512\,94$ Ry and $\Gamma_a=0.009\,518\,7$ Ry for $e+Xe^{53+}$. In Fig. 1 we show the real and the imaginary parts of the scaled dipole matrix element for Fe^{24+}

$$D^{(s)}=\left[\frac{6\pi^2z^4(2J+1)}{\omega^3\alpha^3}\right]^{1/2}D , \tag{21}$$

where the photon energy ω is given in Ry, and D is given in a.u. The dipole matrix element is well fitted by taking $D^0=(2.99\times10^{-2}-8.92\times10^{-5}E)i$ and $A=2.97\times10^{-6}-1.76\times10^{-3}i$. These values allow us to reproduce D within 10%. If we do not neglect the real part of D^0, the fitting becomes even more satisfactory. In general, the real part of D has one maximum and one minimum. In the present case, however, the real part of A is very small, and consequently the minimum cannot be seen clearly.

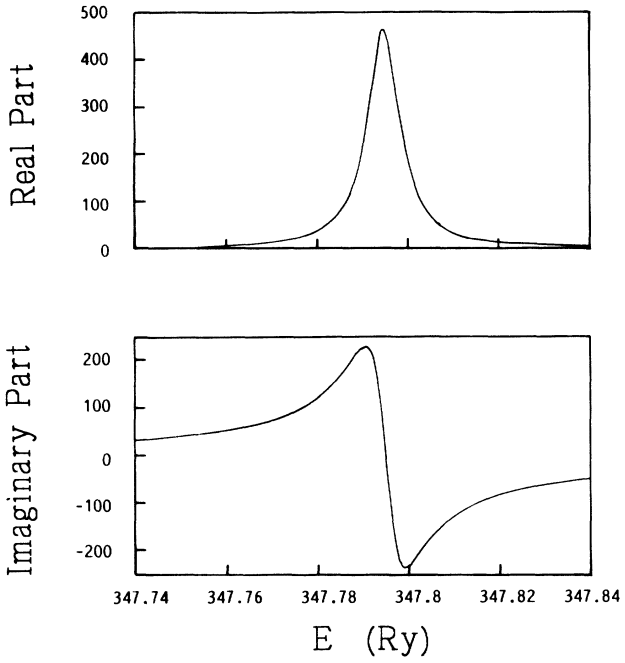

FIG. 1. Real and imaginary parts of scaled dipole matrix elements $D^{(s)}$, defined in Eq. (21), for Fe^{24+} as a function of the energy E (in Ry).

Figure 2 compares the photoionization probability (18) and the probability in first-order perturbation theory

$$P_{e\text{-}p}^{(1)}=4\pi^2|D|^2 , \tag{22}$$

for Fe^{24+}. It clearly shows that $P_{e\text{-}p}^{(1)}$ significantly overestimates the probability and even exceeds unity in the region of the resonance. However, away from the resonance, the two results coincide well with each other. This fact means that for highly charged ions, first-order

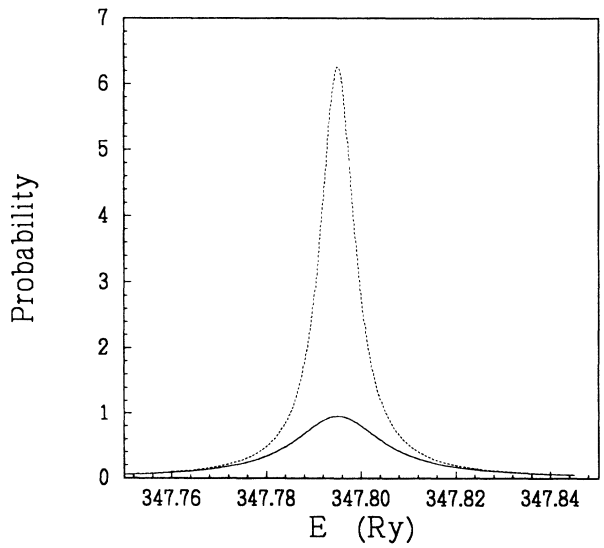

FIG. 2. Probabilities $P_{e\text{-}p}$ (solid line) and their first-order approximation $P_{e\text{-}p}^{(1)}$ (dotted line), defined in Eqs. (18) and (22), for Fe^{24+} as a function of the energy E (in Ry).

perturbation theory is applicable to the direct process but not to the process occurring through the resonance.

The resonance structure is a simple Lorentz form, and has no remarkable interference effect. The background (nonresonant contribution) is very small compared to the resonant contribution. Neglecting D^0 and setting

$$\Gamma_r = 4\pi^2 \frac{|A|^2}{\Gamma_a} , \tag{23}$$

we have

$$P_{e\text{-}p} = \frac{\Gamma_a \Gamma_r}{(E-E_a)^2 + \frac{1}{4}(\Gamma_a+\Gamma_r)^2} . \tag{24}$$

Thus the total width is given by $\Gamma = \Gamma_a + \Gamma_r$, and Eq. (23) is regarded as the definition of the width due to the radiation. In the present case $\Gamma_r = 0.0138$ Ry, which is comparable with Γ_a. Hahn and LaGattuta[7] calculated Γ_a and Γ_r for the same process by using a Hartree-Fock code in both *LS* and intermediate coupling schemes (Appendix B in their paper). Relativistic calculations were also presented by Vainstein and Safronova[11] and Dubau *et al.*[12] All these calculations employ the distorted-wave-type method, and neglect the nonresonant contribution. The results are summarized in Table I. The results of Hahn and LaGattuta indicate that relativistic effects are not so important for this process in Fe^{24+}. Furthermore, the present calculation shows that the nonresonant contribution is negligibly small. Consequently, all the results presented in Table I are in reasonable agreement with each other.

In Fig. 3, we present the probability $P_{e\text{-}p}$ for Xe^{52+}. The maximum value of $P_{e\text{-}p}$ is about 0.1, which is much smaller than that for Fe^{24+}. In the case of Xe^{52+}, one expects that the radiation-damping effect becomes very important. Figure 3 shows that first-order perturbation theory gives a maximum probability of one hundred. This is an extraordinarily large value, and it indicates that first-order perturbation theory has no meaning at all. However, away from the resonance, first-order perturbation theory is applicable, as in the case of Fe^{24+}. Using Eq. (23), we have $\Gamma_r = 0.256$ Ry which is 27 times larger than Γ_a (=0.009 52 Ry). Hence the total width of the resonance for Xe^{52+} is almost equal to Γ_r. We must include relativistic effects in order to obtain an accurate result for Xe^{52+}. However, we believe that the qualitative result remains valid even without inclusion of the relativistic effects.

TABLE I. Calculated widths (in Ry) for the $2s2p\ ^1P$ state of Fe^{24+}.

	Γ_a	Γ_r
Present work	0.008 83	0.0138
Ref. 7 (*LS*)[a]	0.009 20	0.0134
Ref. 7 (IC)[b]	0.008 90	0.0134
Ref. 12	0.008 26	0.0125
Ref. 11	0.009 43	0.0134

[a] *LS* denotes *LS* coupling scheme.

[b] IC denotes intermediate coupling scheme.

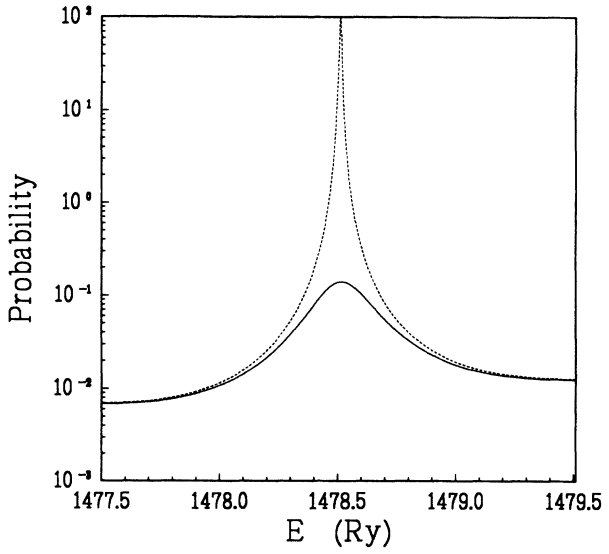

FIG. 3. The same as in Fig. 2 except for Xe^{52+}.

IV. SUMMARY AND DISCUSSION

The present work provides a method to calculate accurately the *S* matrix including radiative channels. Both resonant and nonresonant contributions are included without any significant approximations. The dipole matrix elements are fitted to the form (12). The fitting is easy when the resonance is isolated. However, for overlapping resonances, it may be difficult, and one needs another way to evaluate the integral (5).

The radiation-damping effect is very important when the scattering process of a highly charged ion involves a resonance. Accordingly, we cannot use first-order perturbation theory to calculate photoinduced autoionization and dielectronic recombination probabilities. (It should be noted that radiative recombination is the reverse process of photoionization.)

As the ion charge increases, the total rate coefficient of direct radiative recombination becomes larger than that of dielectronic recombination.[13] This suggests that the interference between the dielectronic and the direct radiative recombination becomes important for a highly charged ion.[14,15] However, for the process (15), the nonresonant contribution is still negligibly small for Xe^{52+}. If we scale the present results along the isoelectronic sequence, the non-resonant contribution probably becomes important only for $z > 100$. It requires a further study to see whether the interference effect is actually negligible or not for processes other than (15).

The radiation effect is very important in the electron-impact-excitation (e-e) process of a highly charged ion.[16–20] Pradhan and Seaton[19] studied its effect on the structure of high-lying resonances by using a quantum-defect theory.[3] The present method can be applied to study the effect for low-lying resonances. The work is now in progress. We will also extend our method to include relativistic effects.

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