Effect of Dielectronic Recombination on Electron-Ion Scattering Cross Sections

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It is shown that the loss of electron scattering flux through dielectronic recombination can be quite significant for highly charged ions, thus reducing the contribution of autoionizing resonances to scattering cross sections and hence excitation rates. This process is likely to be of importance in analyzing line emission from high-temperature plasmas. Detailed calculations are carried out for O^{6+} and Fe^{24+}. Employing the present formulation, the averaged cross sections for dielectronic recombination may also be computed.

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Electron impact excitation (EIE) of positive ions and dielectronic recombination are important atomic processes in laboratory and astrophysical plasmas. Accurate rate coefficients are required for diagnostics and other purposes such as power loss from nuclear fusion reactors, cooling rates for astronomical objects, etc. In recent years electron-ion scattering calculations for multiply charged ions have shown that the Rydberg series of autoionizing resonances in the cross sections often make a large contribution to excitation rates—resulting in enhancements by significant factors in comparison with nonresonant calculations.[1-4] We have carried out extensive calculations (Refs. 3 and 4, referred to as Papers I and II) for the detailed cross sections and rate coefficients for a number of heliumlike ions from Be^{2+} to Fe^{24+}. It was found that the resonance structures in the cross sections for a numbers of transitions were large enough to enhance the effective rate coefficients by up to a factor of 5 or more at temperatures close to those for the maximum abundance of the ions. This is true of nearly all the weak forbidden transitions whose line-intensity ratios are particularly important for diagnostics.

Dielectronic recombination (DER) is a process whereby an incident electron with insufficient energy to excite a given ionic state, becomes trapped in an autoionizing level belonging to that state followed by radiative decay of the excited state, which usually corresponds to an optically allowed transition. As the transition probability is proportional to Z^4, it is clear that DER would become an increasingly important mechanism with increasing Z. The processes of EIE and DER are thus related through autoionization (see the review by Seaton and Storey[5]). The first calculation of electron-ion scattering cross sections, taking the effect of DER into account, was carried out by Presnyakov and Urnov[6] for O^{5+}. In the present work we adapt and extend their approach employing a quantum defect theory formalism developed by Gailitis[7] and Seaton,[8] and thereby compute detailed collision strengths including resonance structures, collision strengths averaged over resonances, averaged collision strengths taking DER into account, and, finally, contributions to the collision strength for DER.

The collision strength is related to the scattering matrix $\underline{S}$ as

$$\Omega_{if}^{SLp} = \tfrac{1}{2}(2S+1)(2L+1)\sum_{l_i,l_f} |S(S_iL_il_i;S_fL_fl_f)|^2, \quad (1)$$

where S_iL_i and S_fL_f are the initial and final target states, l_i and l_f are the initial and final orbital momenta of the scattering electron, and SLp is the total symmetry of the e + ion system with S being the total spin, L the total orbital angular momentum, and p the parity of the system. Multichannel quantum defect theory (MCQDT) as developed by Gailitis and Seaton deals with the threshold behavior of the $\underline{S}$ matrices when a number of channels are to be considered. For all channels open one may define a matrix $\underline{\chi}$ such that $\underline{\chi}=\underline{S}=(i-\underline{R})(i+\underline{R})^{-1}$, where $\underline{R}$ is the reactance matrix which has the advantage of being real and is generally the quantity that is computed in scattering calculations. When some channels are open and some closed, we may partition $\underline{\chi}$ as $\underline{\chi}_{oo}$, $\underline{\chi}_{oc}$, $\underline{\chi}_{co}$, and $\underline{\chi}_{cc}$, where o and c refer to open and closed channels, respectively. Diagonalizing the submatrix $\underline{\chi}_{cc}$, and performing contour integration over the poles corresponding to the Rydberg series of resonances below threshold, one obtains the following expression, derived by Gailitis, for the averaged $\underline{S}$ matrix elements:

$$\langle |S_{\alpha\beta}|^2\rangle = |\chi_{\alpha\beta}|^2 + \sum_{n,m} \frac{\chi_{\alpha\beta}\chi_{n\beta}\chi_{\alpha m}^*\chi_{m\beta}^*}{1-\chi_{nn}\chi_{mm}^*}, \quad (2)$$

where n,m refer to closed channels and α,β to open channels. Equation (2) may be expanded as

$$\langle|S_{\alpha\beta}|^2\rangle = |\chi_{\alpha\beta}|^2 + \sum_{n=m=1}^{M} \frac{|\chi_{\alpha n}|^2|\chi_{n\beta}|^2}{\sum_\gamma|\chi_{n\gamma}|^2} + 2\,\mathrm{Re}\left(\sum_{n\neq m} \frac{\chi_{\alpha n}\chi_{n\beta}\chi_{\alpha m}^*\chi_{m\beta}^*}{1-\chi_{nn}^*\chi_{mm}^*}\right). \quad (3)$$

In deriving (3) we have made use of the unitarity of the $\underline{S}$ matrix and the fact that χ_{cc} is diagonal, i.e., $1-|\chi_{nn}|^2 = \sum_\gamma|\chi_{n\gamma}|^2$, where γ refers to all the open channels. The second term in (3) is a sum over all the closed channels (M) and represents the probability of capture $|\chi_{\alpha n}|^2$ into a resonance state corresponding to the nth closed channel, and subsequent autoionization probability $|\chi_{n\beta}|^2/\sum_\gamma|\chi_{n\gamma}|^2$. The last term in (3) represents interference effects between the closed channels and is usually quite small. The MCQDT, partly sketched above, has been incorporated into a computer program[9] RANAL that analyzes the reactance matrices and computes detailed and averaged collision strengths. In atomic units we may write the autoionizing probability as $\Gamma_A(\nu) = z^2/2\pi\nu^3\sum_\gamma|\chi_{n\gamma}(\nu)|^2$, where ν is the effective quantum number corresponding to the nth closed channel and z is the ion charge. The radiative transition probability is given by $\Gamma_R(i,j) = 2(\Delta E_{ij})^2 \times \alpha^3(\omega_i/\omega_j)f_{ij}$, where ΔE_{ij} is the energy difference between the levels i and j ($\Delta E_{ij} \propto Z^2$), ω_i and ω_j their statistical weights, f_{ij} the absorption oscillator strength, and α the fine-structure constant. We now replace the pure autoionization term in the Gailitis expression (3), by a branching ratio between autoionization and radiative decay. This simply involves the substitution

$$\sum_\gamma|\chi_{n\gamma}|^2 \to \sum_\gamma|\chi_{n\gamma}|^2 + \frac{2\pi\nu^3}{z^2}\Gamma_R(i,j) \quad (4)$$

in the denominator of the second term on the right-hand side of Eq. (3). The levels i and j in (4) represent the core states of the *target* ion (the scattering electron is assumed to be sufficiently far from the core not to be able to perturb the transition significantly). In the present work we consider DER corresponding to optically allowed core transitions (forbidden transitions may also occur). Equation (4) is based on a similar approach by Presnyakov and Urnov.[6] The interference term in Eq. (3) has been shown by Seaton[10] to be not very important in practical calculation and radiative corrections to this last term have been ignored. With the substitution of (4) into Eq. (3), the $\underline{S}$ matrix elements no longer satisfy the unitarity condition due to loss of flux into the DER channels. However, if one takes into account the recombining electron flux, then it follows from unitarity and the Gailitis threshold law that the total scattering *and* recombination cross section just below a given threshold must equal the total cross section just above. If we denote the left-hand side of Eq. (3) with the substitution (4) as $\langle|S_{\alpha\beta}|^2\rangle_d$, then for an incident channel α and outgoing channel β,

$$\langle|S_{\alpha\beta}|^2\rangle - \langle|S_{\alpha\beta}|^2\rangle_d = \sum_b\langle|S_{\alpha b}|^2\rangle_{\mathrm{DER}} \quad (5)$$

where the right-hand side represents the probability of recombination to the final e + ion bound states b, and is related to the DER collision strength averaged over contributions from resonances below threshold.

The scattering calculations are described in detail in Paper I. We solve the e + ion scattering problem in the distorted-wave (DW) approximation in which the coupling between states, other than the initial and the final, is neglected (for heliumlike ions the DW results are in very good agreement with the close-coupling results, ~10%). We include the ground state and all the excited $n=2$ states, i.e., 1^1S, 2^3S, 2^3P°, 2^1S, 2^1P°, in the e + ion wave function expansion. The energy range of interest in this work includes the region up to the $n=2$ states, where we use MCQDT in order to analyze the resonance structures. Calculations are carried out for the $\underline{R}$ matrices in the region just above the 2^1P° state where these matrix elements are found to be fairly smoothly varying. Extrapolation of the $\underline{R}$ matrices to energies below the $n=2$ thresholds yields the detailed collision strengths with resonances, according to the following expression[8]:

$$\overline{\underline{R}}_{oo} = \underline{R}_{oo}^< - \underline{R}_{oc}^<(\underline{R}_{cc}^< + \tan\nu_c)^{-1}\underline{R}_{co}^<, \quad (6)$$

where $\overline{\underline{R}}$ is the reactance matrix below threshold where some channels are open and some closed. The superscript "<" indicates that these matrices are obtained by making an analytic continuation of the $\underline{R}$ matrix computed above threshold, to energies below. The Gailitis averaging procedure as described in the previous section yields the averaged collision strengths from the extrapolated $\underline{R}^<$ matrices. We consider inelastic transitions from the ground state 1^1S to the $n=2$ states and compute the effect of recombinations followed by the allowed core transition $2^1P^\circ \to 1^1S$. Thus we allow for the radiative decay of autoionizing states of the type $2^1P^\circ nl$ that occur as resonances in the collision strengths for the inelastic transitions 1^1S-2^3S, $1^1S-2^3P^\circ$, and 1^1S-2^1S. The radiative probabilities are computed from the most accurate oscillator strengths available: $f(2^1S-2^1P^\circ)=0.703$ for Fe^{24+} (Wiese[11]) and 0.694 for O^{6+}.[12] The energy difference $\Delta E(2^1P^\circ-1^1S)$ is 11.3159 a.u. for O^{6+} and 244.0114 a.u. for Fe^{24+} (Paper I). It is known from our earlier scattering calculations that nearly all the contribution to the collision strengths for the above transitions is from partial waves $l_i, l_f \leq 4$ [Eq. (1)] (contributions from $l_i, l_f > 4$ are less than 5% of the total and are neglected). The symmetries of the e + ion system (denoted by SLp) corresponding to the partial waves included are ^2S, $^2P^\circ$, ^2D, $^2F^\circ$, and ^2G. Calculations are carried out at two or three energies just above the 2^1P° threshold and the $\underline{R}$ matrices obtained are analyzed using the program RANAL (modified to include the branching between autoionization and radiative decay). In the energy region $E(2^3S)-E(2^3P^\circ)$, the total inelastic cross section is simply the cross section for the transition 1^1S-2^3S with resonances of the type $2^3P^\circ nl$, 2^1Snl, and $2^1P^\circ nl$; whereas in the region $E(2^1S)-E(2^1P^\circ)$ we have three transitions to consider: 1^1S-2^3S, $1^1S-2^3P^\circ$, and 1^1S-2^1S, all with resonances of the type $2^1P^\circ nl$ in their cross sections. The region $E(2^3P^\circ)-E(2^1S)$ is small and is not considered.

In Fig. 1 we present some results for electron scattering with O^{6+} and in Fig. 2, for Fe^{24+}. Each figure consists of three plots: (i) the detailed collision strength showing resonance structures present; (ii) the collision strength averaged over resonances, $\langle\Omega\rangle$, and (iii) averaged collision strength allowing for radiative decay, $\langle\Omega\rangle_d$. The difference between the $\langle\Omega\rangle$ and the $\langle\Omega\rangle_d$ thus represents the decrease in the resonance enhancement of the inelastic cross section due to radiative decay of the autoionizing states $2^1P^\circ nl$. It may be seen that this decrease is quite significant and is a measure of the incident electron flux that goes into dielectronic recombination. The averaged collision strength for DER may now be computed. For example, in the energy region $E(2^1S)-E(2^1P^\circ)$, the DER collision strength $\langle\Omega_{\rm DER}\rangle$ is given by

$$\langle\Omega_{\rm DER}(2^1P^\circ nl\to 1^1Snl)\rangle = \sum_{S_i\,L_i}[\langle\Omega(1^1S-S_iL_i)\rangle-\langle\Omega(1^1S-S_iL_i)\rangle_d], \qquad (7)$$

where $S_iL_i=2^3S$, 2^3P°, and 2^1S. Just below the 2^1P° threshold $\langle\Omega_{\rm DER}\rangle$ must be equal to $\Omega(1^1S-2^1P^\circ)$ extrapolated from just above 2^1P°, as the flux going into the open 2^1P° channels is equal to the flux previously (below 2^1P°) trapped in the closed channels $2^1P^\circ nl$ and going into DER. Also at the 2^1P° threshold, each of the $\langle\Omega(1^1S-S_iL_i)\rangle_d$ continues smoothly over to $\Omega(1^1S-S_iL_i)$ above the threshold [Figs. 1(b), 1(c), and 2], i.e., there is no Gailitis jump. This is because the resonance states just below 2^1P° have very long lifetimes and decay radiatively. As the nuclear charge increases the ratio of the radiative to autoionization probabilities behaves as $Z^4(\alpha\nu)^3$. Thus the ratio Γ_R/Γ_A is considerably larger in magnitude for Fe^{24+} than for O^{6+}. We compute $\Gamma_R/\Gamma_A=(2\pi\nu^3/z^2)\Gamma_R/\sum_\gamma|\chi_{n\gamma}|^2$, at the energy $k^2=E(2^1S)$ (where $\nu\approx 8$)

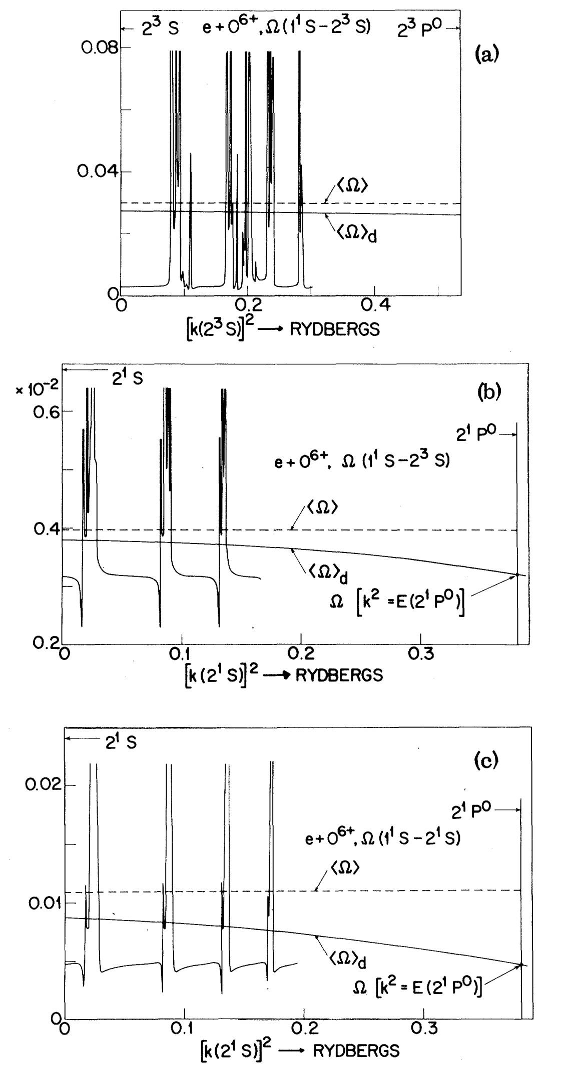

FIG. 1. Collision strengths for electron impact excitation of O^{6+}: (a) transition 1^1S-2^3S, energy range $E(2^3S)-E(2^3P^\circ)$; (b) transition 1^1S-2^3S, energy range $E(2^1S)-E(2^1P^\circ)$; (c) transition 1^1S-2^1S, energy range $E(2^1S)-E(2^1P^\circ)$.

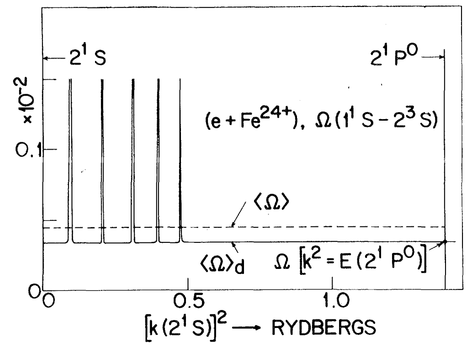

FIG. 2. Collision strengths for electron impact excitation of Fe^{24+}, transition $1^1S - 2^3S$, energy range $E(2^1S) - E(2^1P^\circ)$.

and again at an energy just below $E(2^1P^\circ)$ for Fe^{24+}, $SLp = {}^2S$. We find that $\Gamma_R/\Gamma_A \gtrsim 60$ at the former energy and > 1000 at the latter [on the other hand, this ratio is found to vary only from 0.1 to 0.36 for O^{6+} at energies between $E(2^3S)$ and $E(2^3P^\circ)$]. The effect of this is clearly seen in Fig. 2 where we find that the $\langle\Omega\rangle_d$ coincides almost exactly with the background collision strength for $1^1S - 2^3S$ in the energy region shown, i.e., there is no resonance enhancement of the cross section. Another way to interpret this result is that the autoionization states shown in Fig. 2 would not be seen experimentally in the scattering cross sections, since their radiative probability is much higher than their autoionization probability.

Finally, we note that the effect of DER is found to be considerable and we estimate from the figures given that the effective cross sections could be reduced by about 10–30% due to the decrease in the resonance enhancement from autoionizing states. Work is in progress on a number of aspects of the present topic, in particular, on the effect on excitation rates (Paper II), DER through the forbidden levels,[13] departure from LS coupling[14] and computation of the DER cross sections (including the elastic scattering region). We might point out that calculations or experiments for DER cross sections have not yet been done, though some experiments are now in progress.[15]

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