Electron-Ion Recombination in the Close-Coupling Approximation

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A computational formalism is presented to obtain total electron-ion recombination cross sections and rate coefficients employing the close-coupling approximation for photoionization and scattering and the Bell and Seaton theory of dielectronic recombination. The results differ significantly from separate treatments of the two processes, radiative and dielectronic recombination. The R-matrix method, as developed for the Opacity Project, is used and results are presented for recombination collision strengths and rate coefficients for boronlike O^{2+} and Ne^{4+}.

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The total rate of electron-ion recombination is important in the determination of the ionization structure of laboratory and astrophysical plasma sources where stabilization occurs as a balance between effective ionization and recombination. Diagnostics of nuclear fusion plasmas and spectral formation in astronomical objects require accurate computations for the rates of these atomic processes. Electron-ion recombination is usually considered as two separate processes: radiative and dielectronic (RR and DR); the former is defined as the detailed balance inverse of the background bound-free continuum, i.e., direct photoionization (PI), and the latter as the inverse of autoionization (i.e., radiationless capture) followed by radiative decay. Thus the calculation of $e+$ion recombinations is carried out in two corresponding parts, one involving PI cross sections *without* autoionizing resonances [1,2], and the second involving calculations of autoionization and radiative decay rates [3,4] *independent of each other.* However, the interaction with the background continuum and the effect of overlapping series of resonances may both significantly influence the effective autoionization and hence the recombination rate. It has been pointed out by the authors [5] (hereafter NP1) that PI cross sections calculated in the close-coupling (CC) approximation, with detailed autoionization profiles of series of resonances, may be employed to treat total, effective $e+$ion recombination without the physically artificial distinction between the two processes. During the previous decade there has been considerable activity in the study of DR, both experimentally [6–8] and theoretically [9–13]. In particular, a precise *ab initio* theory of DR has been presented by Bell and Seaton [9] (hereafter BS) as an extension of multichannel scattering theory. Also during the last decade the R-matrix method [14] was extended substantially for radiative and collisional work for $e+$ion systems, in particular for radiative calculations involving arbitrarily excited states, and employed for large-scale calculations under the Opacity Project [15,16]. Combined with the work reported in NP1, the present work incorporates the BS theory within the R-matrix framework to obtain total $e+$ion recombination cross sections and rates.

We consider the $e+$ion system with N electrons in the target ion and $N+1$ electrons in the recombined ion. The recombination problem is divided into a "low-n" part, referring to bound states of the recombined ion with low principal quantum number that may contain a large component of the RR type, and a "high-n" part where DR dominates RR. The low-n recombination requires the calculation of PI cross sections for *all* bound states of the $e+$ion system with $n \le n_0$, where n_0 is a practical limit within which all states are treated with detailed R-matrix calculations. As the R-matrix calculations involve autoionization structures in PI cross sections in an *ab initio* manner, detailed balance yields the total recombination cross section, for the states with $n \le n_0$, through the associated bound-free continua attenuated by the autoionizing resonances. The high-n component, $n_0 < n \le \infty$, consists predominantly of DR through the several infinite series of resonances that converge onto the excited states of the target or core ion included in the CC approximation; it is the latter that is addressed by the BS theory which, based on quantum defect theory, should be particularly valid for high n where the outer electron may be reasonably treated as a "spectator."

The BS theory includes radiation damping in electron-ion scattering that yields an extended scattering matrix $\mathcal{S}$ which is partitioned into submatrices of coupled radiative and scattering channels as $\mathcal{S}_{ee}$, $\mathcal{S}_{ep}$, $\mathcal{S}_{pe}$, and $\mathcal{S}_{pp}$; $\mathcal{S}_{ee}$ gives the electron-ion scattering amplitudes including radiative decay, and $\mathcal{S}_{pe}$ gives the probability amplitudes for electron recombination with photon emission; $\mathcal{S}_{ep}$ refers to the inverse of $\mathcal{S}_{pe}$, i.e., photoionization, and $\mathcal{S}_{pp}$ to photon-photon scattering. The unitarity condition $\mathcal{S}_{ee}^{\dagger}\mathcal{S}_{ee}+\mathcal{S}_{pe}^{\dagger}\mathcal{S}_{pe}=1$ is satisfied for the total electron and photon flux and yields the DR probabilities, given by $\mathcal{S}_{pe}^{\dagger}\mathcal{S}_{pe}$,

$$P_i(\mathrm{DR}) = \sum_{\beta\mu} |\mathcal{S}_{\beta\mu,i}|^2 = (1-\mathcal{S}_{ee}^{\dagger}\mathcal{S}_{ee})_{ii} = 1 - \sum_{j=1}^{\mathrm{NCHOP}} |\mathcal{S}_{ee}(i,j)|^2, \quad (1)$$

where the scattering matrix elements include radiation damping, i is the incident channel, $\beta\mu$ refers to the final bound states β of the $e+$ion system with emission of a photon with polarization μ, and j is the index summing over all NCHOP outgoing scattering channels that are open. The expressions for the elements of the $\mathcal{S}_{ee}$ are obtained in terms of a matrix χ which is the scattering matrix, *without* radiative decay, in the region of all channels open but which is partitioned in the region below threshold into open and closed channel submatrices χ_{oo}, χ_{oc}, χ_{co}, and χ_{cc}. The BS theory then gives the following expressions for the detailed energy behavior and the resonance-averaged quantities by including factors that incorporate the radiative couplings:

$$\mathcal{S}_{ee}(v)=\chi_{oo}-\chi_{co}[\chi_{cc}-g(v)\exp(-2i\pi v)]^{-1}\chi_{co}\,, \quad (2)$$

where v is the effective quantum number in the closed channels, $g(v)=\exp(\pi v^3 A_r/z^2)$, and A_r is understood to be the sum over all radiative transition probabilities for the available decay routes from a given excited state of the target ion. The scattering matrix elements averaged over resonances are obtained as

$$\langle|\mathcal{S}_{ij}|^2\rangle=|\chi_{ij}|^2+\sum_{p\neq q}\frac{\chi'_{ip}\chi'_{pj}\chi'_{iq}{}^*\chi'_{qj}{}^*}{G(v)+1-\chi'_{pp}\chi'_{qq}{}^*}\,, \quad (3)$$

where $G=g(v)-1$. The matrix χ_{cc} is diagonalized as $\chi'_{cc}=\mathbf{X}^T\chi_{cc}\mathbf{X}$; then $\chi'_{co}=\mathbf{X}^T\chi_{co}$, $\chi'_{oc}=\chi_{oc}\mathbf{X}$, where $\mathbf{X}$ is the diagonalizing matrix. In the approximate formulas employed prior to the BS theory, the factor G is intuitively taken to be $2\pi v^3 A_r/z^2$ and radiative corrections to the interference term $p\neq q$ are neglected [17,18].

In NP1 we described the PI calculations for large numbers of bound states of e+ion systems in the carbon isoelectronic sequence with the eventual aim of calculating total recombination cross sections, complemented by the BS theory. A large number of e+ion bound states need to be considered. We calculate the PI cross sections for all bound states, 252 for O^{2+} and 314 for Ne^{4+}, with $n\leq n_0=10$. It is also important to fully obtain and delineate the autoionizing resonances lying close to the ionization threshold as these, if present, may enhance the DR-type component of recombination significantly (referred to as low-temperature DR by Nussbaumer and Storey [3], hereafter NS). Therefore for each bound state the calculations are carried out at several thousand energies to delineate all resonances in the Rydberg series belonging to each excited state of the target ion up to effective quantum number $v=10.0$ corresponding to $n_0=10$. Resonances in PI cross sections with $v>10.0$ are averaged over using the Gailitis method. For states of the recombined ion with $n>n_0$, recombination through the background bound-free continua is negligible, of the order of 1%, and the recombination proceeds predominantly through DR.

The R-matrix code dealing with the calculation of e+ion continuum wave functions and scattering matrices, STGF [16], has now been extended to include radiation damping as described above and used to calculate the DR contribution for $n>n_0$. The DR probabilities for all elastic and inelastic channels leading to the ground state are obtained in detail as a function of v and averaged over the Rydberg series of resonances. Collision strengths for DR for elastic and inelastic scattering including radiative decays are obtained by summing the probabilities over the available channels and total spin and angular symmetries, $SL\pi$, of the e+ion system. Recombination channels leading to excited states of the ion but not connected to the ground state via a dipole transition (i.e., DR thorough forbidden transitions) are ignored.

The eigenfunction expansion for the B-like systems O^{3+} and Ne^{5+} includes eight states: $2s^2 2p(^2P^o)$, $2s2p^2(^4P,^2D,^2S,^2P)$, and $2p^3(^4S^o,^2D^o,^2P^o)$. Radiative channels for all dipole transitions in the ion are included; the ones corresponding to the ground state are $^2P^o\rightarrow{}^2D$, $^2P^o\rightarrow{}^2S$, and $^2P^o\rightarrow{}^2P$. The e+ion scattering calculations include partial waves with $l\leq 9$ and all $SL\pi$ states coupled with the target eigenstates. The threshold collision strengths for the excitation of the allowed transitions are found to have converged with respect to l. The resonance-averaged DR collision strengths using the BS theory, $\langle\Omega(\mathrm{DR})\rangle$, are given in Figs. 1(a) and 1(b) for the recombined ions O^{2+} and Ne^{4+}, respectively.

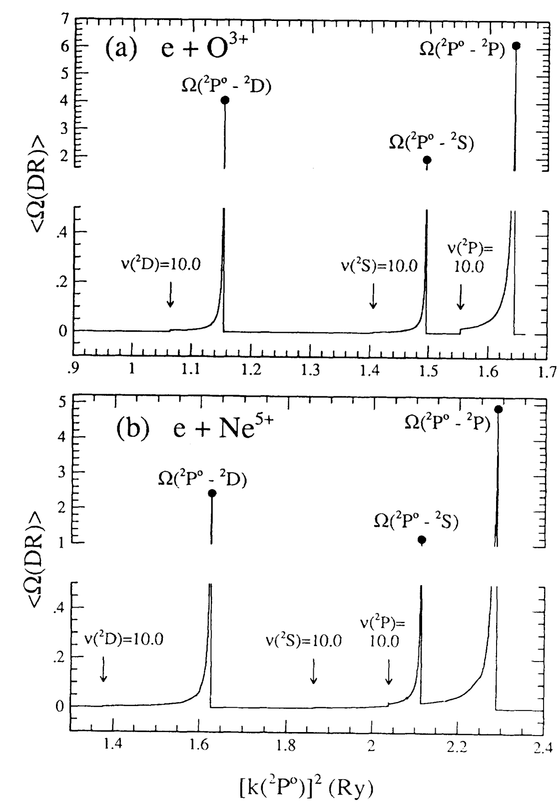

FIG. 1. Resonance-averaged DR collision strength, $\langle\Omega(\mathrm{DR})\rangle$, for (a) O^{2+} and (b) Ne^{4+}. Solid circles represent threshold collision strength for dipole transitions as labeled. The arrows mark $\langle\Omega(\mathrm{DR})\rangle$ values at $v_c=10.0$ of Rydberg series with respect to the ^2D, ^2S, and ^2P states, respectively.

Ne^{4+}, respectively. (The detailed DR collision strengths consist only of δ-function-type features and are not given here.) In the figures the solid circles represent the excitation collision strengths for dipole allowed transitions. The peaks in $\langle\Omega(\mathrm{DR})\rangle$ occur precisely at the threshold excitation energies and the limiting values approach the excitation collision strengths at the threshold. The χ matrices in the region just below threshold (i.e., the Gailitis averaging region) are obtained neglecting long-range multipole (nondipole) potentials in the asymptotic region. The difference in the threshold values of the DR collision strength, with and without the non-Coulomb term, is expected to have only a small effect on the recombination rate coefficients (this is currently being studied). The range of energies considered begins at $\nu=10.0$ and the very slight rise in the DR collision strengths at those points indicates their magnitude at approximately $n_0=10$; i.e., most of the DR contribution is concentrated just below the threshold(s) of convergence. In the multichannel calculations the DR collision strengths need not in fact be limited by the threshold excitation collision strengths since there may be DR contributions from closed channels belonging to several target states higher than the one corresponding to the allowed transition. This is the case for $e+Ne^{5+}\rightarrow Ne^{4+}$ at energies just below $E(^2S)$. At $E(^2S)$, $\nu=11.8$ relative to $E(^2P)$; therefore with $\nu=10.0$ the averaged DR collision strengths below ^2S have a small contribution from the ^2P channels. Although not significant in the present cases, it could assume greater importance in ions where several closely spaced allowed transitions contribute to DR in a given energy region.

In Figs. 2 and 3 we present the Maxwellian-averaged total recombination rate coefficients, α_R, including the contributions from all states, $n\leq\infty$, of the recombined ion at temperatures of interest for equilibrium plasmas for O^{2+} and Ne^{4+}. For O^{2+}, comparisons are made with the low-temperature DR rate coefficients by NS [3], the high-temperature DR rate coefficients of Badnell and Pindzola [4], the RR rate coefficients by Aldrovandi and Pequignot [1], and the DR-only contribution from the BS theory for $10<n\leq\infty$. The present results, representing the combined, effective $e+$ion recombination (solid curve), yield values in the entire temperature range unlike previous works. In particular, the results show that in the *intermediate-temperature* range the previous results, based on a *separate* consideration of the two processes, underestimate the recombination rate significantly. For example, the present value at $\log_{10}T=4.7$ is higher than the *sum* of the RR and the DR (NS) value by 70%. In this temperature range the recombination through the background bound-free cross sections (RR-type), in the near ionization threshold region, is still significant while that through the converging autoionizing resonances at higher energies has not yet begun to mani-

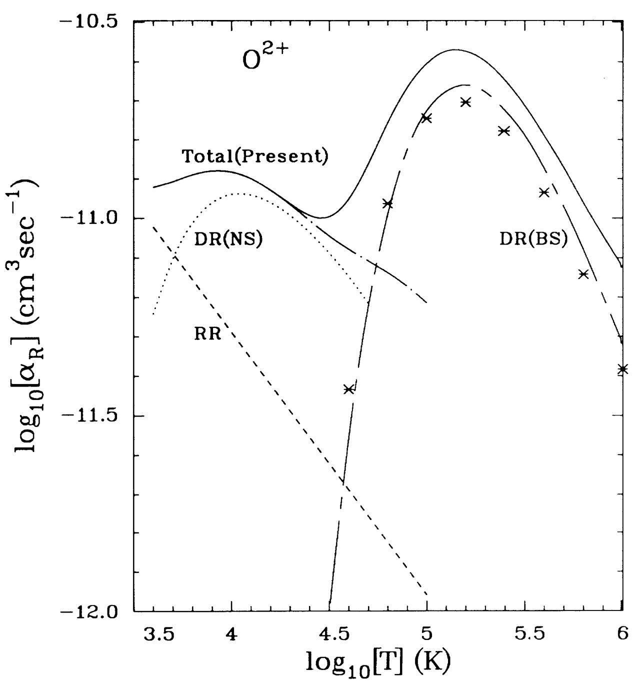

FIG. 2. Total recombination rate coefficients, α_R, for O^{2+} (solid curve). The dotted-chain curve corresponds to the "low-n" part, $n\leq 10$; the dashed-chain curve is the "high-n" part, $10<n\leq\infty$, consisting of DR contribution according to BS theory; the dashed curve represents RR contribution [1] and the dotted curve low-temperature DR contribution by NS [3]; the asterisks are the DR rate coefficients of Ref. [4].

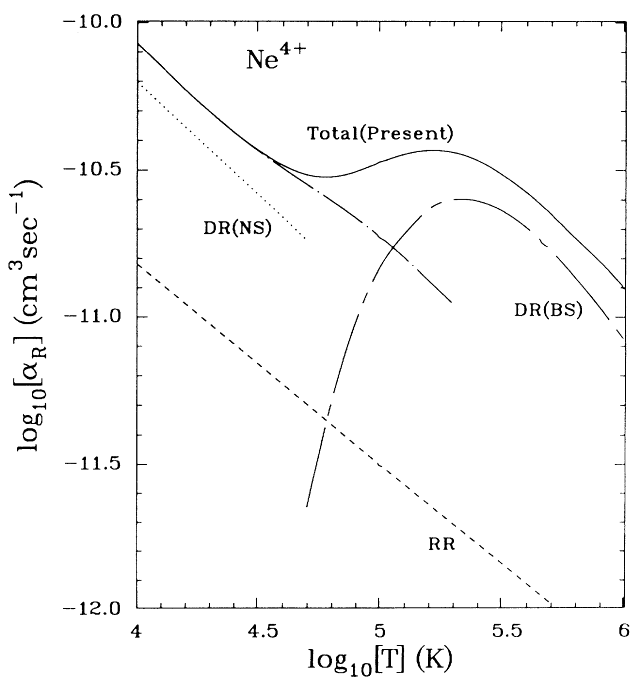

FIG. 3. Total recombination rate coefficient, α_R, of Ne^{4+} (solid curve); the other curves are as for Fig. 2.

fest itself. Thus the usual practice of summing the two rates, RR+DR, does not adequately describe this region. The present results, on the other hand, include not only the background PI cross sections (for all possible contributing states) but also all resonances which are coupled together and hence include overlapping structures accounting for the attenuation of the background continua. For example, the present value at $\log_{10}T=4.7$ is higher than the *sum* of the RR and the DR (NS) value by 70%. As pointed out in previous works [4,5], and in NP1, the near threshold autoionizing resonances also make a significant contribution as indicated by the large difference in the rate coefficients between curves labeled RR, DR, and total, resulting in the characteristic low-temperature hump. The low-lying autoionizing resonances do not, however, appear for all ions; the Ne^{4+} rates in Fig. 3 do not exhibit the hump, although the effective rate coefficient is high owing largely to the contribution from the background bound-free continua. Although completely different approximations have been employed in the present calculations *vis-à-vis* the earlier DR (NS) [3] and RR [1] works, the present results agree well in shape with the *sum* of the earlier values, and are about 10% higher in the low-temperature region. The Ne^{4+} results do, however, show the high-temperature rise due to the high-lying resonances converging onto the ^2D, ^2S, and ^2P states of the Ne^{5+} target ion.

In conclusion, we might note that, with the present extension, the CC method provides a self-consistent treatment of electron-ion recombination of atoms and ions, on par with photoionization and electron scattering, given a common eigenfunction expansion in the R-matrix calculations. Further extensions in progress include intermediate coupling effects, both in an algebraic recoupling scheme [19] and in the Breit-Pauli R-matrix method [20], external field effects considered with the BS theory (e.g., by Harmin [21] and Sakimoto [22]), and higher-order effects that may be important for very highly charged ions [23]. The present formulation should yield accurate electron-ion recombination rates and should also provide useful tests for the further development of unified theories of recombination beyond the isolated resonance approximation hitherto employed [12,13].

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