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Investigation of collisional and electric field effects on the He I dielectronic recombination rates for magnetic fusion plasmas

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Abstract

We present numerical calculations for the He I dielectronic recombination rate coefficients which take into account dense plasma effects. Collisional redistribution of the population between the autoionizing levels as well as level depression due to electric fields seriously alter the He I total dielectronic recombination rate. Atomic kinetic population simulations carried out with the SOPHIA code demonstrate that these high density effects influence largely on the ionic/atomic fraction and therefore on all diagnostic interpretations which employ atomic population densities like, e.g., line intensities.

Key words: Dielectronic recombination, dense plasma effects, diagnostics, magnetic fusion plasmas.

I. Introduction

The Dielectronic recombination (DR) begins when a free electron excites a positive ion and is simultaneously captured into an excited state. DR is completed when the recombined atom/ion emits a photon that brings the total energy of the ion below its ionization threshold. DR is a resonant process because it involves the creation of a doubly excited state embedded in the continuum of the electron-ion system.

DR is an important recombination process for magnetic fusion plasmas to describe the radiative properties of atoms and ions. The understanding of this process which goes beyond the traditional calculations in the isolated atom approach is of manifold interest for plasma diagnostics.

In this paper we present our numerical calculations for the He I DR rate coefficient. We show that collisional ionization and level depression due to electric fields, which are preferentially important for large quantum numbers turned out to be of extreme importance for typical parameters of edge plasmas. These effects seriously alter the He I total DR rate. Employing atomic population kinetic calculations we show that via DR collisional effects and level depression modify strongly the atomic/ionic fraction He II and HeI .

II. He I Dielectronic recombination rate coefficient calculations

The calculation of the DR rate coefficients requires complete sets of atomic data, i.e., energies, radiative and autoionization rates. These data have been calculated with the Flexible Atomic Code, FAC [1]. It is based on the relativistic configuration interaction with independent particle basis wave functions. Relativistic effects are taken into account using a Dirac-Coulomb Hamiltonian. Higher order QED effects are included with Breit interaction in the zero energy limit for exchanged photon. Continuum processes are treated in the distorted-wave (DW) approximation. Radiative transition rates are calculated in the single multipole approximation with arbitrary ranks. The calculation of autoionization rates is based on the relativistic DW and isolated resonance approximations, more details are described in ref. [1]

II.1 Low densities

At low density, the isolated autoionizing level satellite intensity factor is defined as:

$$Q_{isol,\,ji} = \frac{g_j \Gamma_j A_{ji}}{\Gamma_j + \sum_i A_{ji}}, \tag{1}$$

where Γ_j is the autoionization rate for the state j, g_j is its statistical weight and A_{ji} is the radiative decay rate coefficient for the transition j → i. The corresponding DR rate coefficient is given by:

$$\langle DR \rangle_{ji} = 1.656\ 10^{-22} \frac{1}{g_s} Q_{isol,ji} \frac{e^{-E_{s,j}/KT}}{(kT)^{3/2}} \left[cm^3 s^{-1}\right] \tag{2}$$

where $E_{s,j}$ is the capture energy for the 2*l*n*l* in eV, kT is the electron temperature in eV and g_s is the statistical weight of the lower state.

We have performed detailed numerical calculations up to n=10 (see table 1) distinguishing different spin states, i.e., 1s2l (^{1}S, ^{3}S, ^{1}P and ^{3}P) and 1snl (^{1}L and ^{3}L). DR for higher quantum numbers were generated by scaling relations which were derived from the numerical calculations for n=2-10. The scaling relations are converging for all spin (S), angular (L) and main (n) quantum numbers [2] (table 1). Our numerical results for the total DR rate coefficient [2] agree well (within 20 %) with the detailed calculations of Burgess and Wang [3,4] while deviations by more than a factor of 2 are visible for other methods [2].

II.2 High densities

At high electron densities where the collisional rates exceed the autoionization and radiative decay rates (Boltzmann limit) all autoionizing levels of one manifold 2lnl' are statistically populated and the corresponding satellite intensity factor takes the form:

$$Q_{Boltz} = \frac{\overline{g}\,\overline{\Gamma}\,(\overline{A}_{21} + \overline{A}_{n1})}{\overline{A}_{21} + \overline{A}_{n1} + \overline{\Gamma}} \tag{3a}$$

$\overline{g}$ is the statistical weight of the manifold 2lnl', $\overline{A}$ and $\overline{\Gamma}$ are the statistically averaged radiative decay and autoionizing rates, respectively. Scaling relations [2] were also used to calculate Q_{Boltz} for large quantum numbers n. Our results for Q_{Boltz} according eq. (3a) are reported in table 1. Collisional redistribution effects result in a considerable increase of the Q-factor because collisions result into an increase in the phase space for DR and therefore the DR is increased. A similar effect is encountered for electric field effects on the DR [5]. For an applied electric field the principal effect on the DR process is to mix states of low *l* (orbital angular momentum number) with states of high *l*, for large n. Since dielectronic capture normally proceeds readily into states of low *l*, but hardly at all into states of high *l* [6], the effect of an applied electric field is to increase the number of intermediate states accessible to DR, and thereby to increase the DR rate coefficient [7].

When considering collisional redistribution effects, collisional ionization from the high n-level leads to a decrease of the DR:

$$Q_{Boltz} = \frac{\overline{g}\,\overline{\Gamma}\,(\overline{A}_{21} + \overline{A}_{n1})}{\overline{A}_{21} + \overline{A}_{n1} + \overline{\Gamma} + I_n} \tag{3b}$$

I_n is the ionization rate coefficient from level n. Collisions result therefore in two effects: first, increase of the DR due to the increase of the phase space for DR and, second, decrease of the DR due to ionization. This approach differs from those applied so far in the literature where the DR for the isolated level approach is modified by an additional factor to account for the ionization processes [8].

Table 1: *Numerical and scaled intensity factors Q_{isol} and Q_{Boltz}*

Config.	Q_{isol}	$Q_{isol,Scale}$	Q_{Boltz} (eq. 3a)	$Q_{Boltz,scale}$
2l2l’	0.16E+12		0.29E+12	
2l3l’	0.67E+12		0.92E+12	0.90E+12
2l4l’	0.65E+12		0.15E+13	0.15E+13
2l5l’	0.56E+12	0.58E+12	0.23E+13	0.23E+13
2l10l’	0.41E+12	0.43E+12	0.47E+13	0.47E+13
2l15l’		0.27E+12		0.24E+13
2l20l’		0.16E+12		0.11E+13
2l30l’		0.65E+11		0.34E+12
2l50l’		0.16E+11		0.74E+11

II.3 Intermediate densities

At intermediate densities, we encounter a mixing of the two high density effects (eqs. 3a and 3b) with the isolated level approach according eq. (1). We can estimate the DR at intermediate densities:

$$Q = \sum_{n=2}^{n_{crit}} Q_{isol} + \sum_{n>n_{crit}}^{n_{\max}} Q_{Boltz} \tag{4}$$

The critical quantum number n_{crit} can be estimated according:

$$I_n(2l n_{crit} l' \rightarrow 2l + e) \approx \overline{A}_{21} + \overline{\Gamma}(n_{crit}) \tag{5}$$

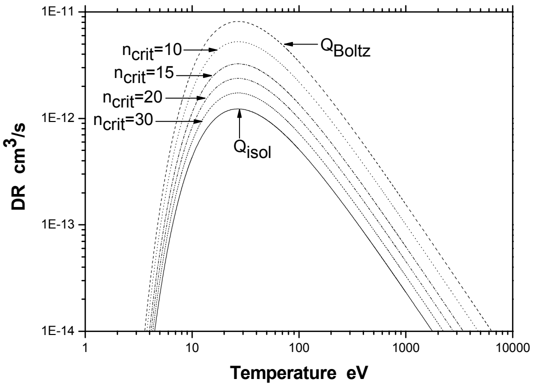

Fig. 1: *DR rate coefficients*

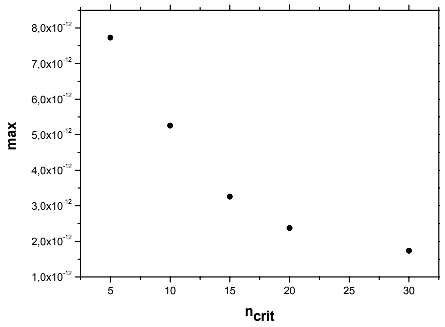

Fig. 2: *Variation of Q_{max} with n_{crit}*

Our DR results are plotted in the fig.1 for different regimes. The DR for the Boltzmann limit according eq. (3a) is more than 6 times larger than the calculated DR for Q_{isol} at the maximum value of the DR rate coefficients (Q_{max}). Therefore, the collisional process between the doubly excited states which are usually neglected are very important. Fig. 2 shows that the Q factor, following eq.(4) depends on the critical main quantum number.

IV. Influence of DR rate coefficient on the atomic/ionic balance

The results in table 1 show a slow convergence of the Q-factor. This circumstance is connected with the low radiative decay rates of neutral atoms and the large autoionizing rate (note, that the radiative decay rates scales with Z^4 whereas the autoionizing rate is essentially independent of Z). Therefore, only at very large quantum numbers the autoionizing rate is of the order of the radiative decay rate. Table 1 shows that DR is far from convergence at those quantum numbers, where the level depression leads to the complete disappearance of n_{max} (the maximum quantum number can be estimated from ref. [9], e.g., for the He I and an electronic density $n_e=10^{14}$ cm^{-3}, $n_{max}=16$.) Therefore, the slow convergence enters critically the DR via collisional redistribution effects and level depression due to electric fields.

Due to variation of the rate coefficients due to different high density effects, the atomic population kinetics code SOPHIA [10] was used to investigate the corresponding effects on the atomic/ionic balance of HeII and HeI. The double ratio R according to [11]:

$$R = \{n(1s^2)/n(1s)\}_{\mathrm{mod}\,el} / \{n(1s^2)/n(1s)\} \qquad (6)$$

can be decreased by a factor of 3 for a simple ground state model, where all DR is coupled into the ground state of He I. A factor of 10 decrease is encountered for a channel collisional model, where all DR is coupled into the respective single excited singlet and triplet states after radiative decay. Therefore, high density effects influence largely on the ionic/atomic fraction via the dielectronic recombination rate and therefore on all diagnostic interpretations which employ atomic population densities.

V. Conclusion

Calculations of the He I DR rate coefficient including dense plasma effects show the importance of collisional redistribution between the autoionizing levels as well as level depression due to electric fields. Simulations carried out with the SOPHIA code show, that inaccuracies of atomic data may enter directly to the inaccuracy of ionic fractions. Moreover, spin dependent channeling of DR rates and collisions influence on the atomic/ionic balance by a factor of 10 and therefore on all diagnostics employing atomic population densities.

VI. References

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