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EFFECT OF EXCITATION-AUTOIONIZATION IN NON-LOCAL THERMODYNAMIC EQUILIBRIUM PLASMAS*

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Based on the detailed configuration accounting model, the authros have developed a method to calculate the rate of excitation-autoionization (EA) in the average atom model and used it in the rate equations. The numerical results show that EA effect is signifficant in high temperature low density plasma and can cause an additional ionization up to 15% of an ionization stage.

Keywords: excitation-autoionization, non-local thernodynamical equilibrium, average atom model
PACC: 5220, 5225

I. INTRODUCTION

It has been long known that it requires non-local thermodynamical equilibrium (non-LTE) models to simulate laser-produced plasmas.[1] The capability to accurately predict atomic level populations is central for us to have the ability to understand and diagnose their radiative properties. Since 1980s, many non-LTE models have been developed.[1−6] These models can be divided into two classes: detailed configuration accounting (DCA) models[1,3,6] and average atom (AA) models.[4,5] The AA models are applied to the simulation in the atomic physics package used in hydrocodes or for high-Z media plasmas, for which DCA models are much complex and time-consuming. For high-Z plasmas, the differences are signifficant even for the results of average ionization stage among these models.[7] Improvement of the accuracy in predicting the atomic level populations is needed. As we know, all the atomic processes in the plasmas affect the level populations, thus it is necessary to include all the important processes in the non-LTE kinetic models. The dielectronic recombination (DR) process proves to have strong influences on the ionization stage[6,8] and its reverse process, called resonant photoionization (RP), is also studied.[9] There is another similar process called excitation-autoionization (EA) which could also be regarded as a kind of reverse process of DR in the environment of plasmas. EA can significantly enhance the total ionization rate and in some cases the rate of EA is larger than that of the direct ionization.[10,11] Djaoui[12] investigated the EA effects on ionization stage distribution and the result is that the fraction of Ni-like ions in tungsten plasmas increases more than four times as including the EA rate for Zn-like and Cu-like ions. Fournier *et al.*[13] also took into account the EA rate for argon plasmas. Both Djaoui and Fournier used DCA models, in which the calcualtion of EA rate is very complicated. However, so far there is not any efficient way to calculate EA for AA models.

The aim of this paper is to develope a method to calculate EA rate for AA models and to investigate the effects of EA on the ionization stage in non-LTE plasmas.

II. THEORY

The contribution of EA to the average population change of the kth subshell can be derived from the rate equations for DCA model if neglecting part of the contribution of excited states

$$c_k \frac{\mathrm{d}p_k}{\mathrm{d}t} = -\overline{\alpha}_k, \tag{1}$$

where c_k and p_k are the statistical weight and the occupation probability of the kth subshell, respectively, $\overline{\alpha}_k$ represents the average EA rate coefficient for the kth shell obtained by averaging over all ionic species in plasmas

$$\overline{\alpha}_k = \sum_{z,n,m} \frac{N_{z,n}}{N} \alpha^{\mathrm{EA}}_{z,n,z+1,m}, \tag{2}$$

where $N_{z,n}$ is the number of the ions in charge state z with an excited or ground electron in the nth level (hereafter we label this ion as (z,n)), $\alpha^{\mathrm{EA}}_{z,n,z+1,m}$ is the EA rate from ion(z,n) to ion$(z+1,m)$.

In the AA model only one configuration is taken into account, that is, the "average ion". For the "average ion", the EA rate coefficient can be written as

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$$\alpha_k^{\mathrm{EA}} = \sum_j \sum_{m<k, m<j} c_m p_m (1-p_j) \alpha_{mj} N_{\mathrm{e}} B(m,j,k), \tag{3}$$

where α_{mj} is the rate coefficient of electron compact excitation from the mth subsheel to the jth subshell, N_{e} is the electron density and E_j the energy of the jth subshell, B is the branch ratio defined as

$$B(m,j,k) = \frac{AA(m,j,k)}{\sum_{k'>m} AA(m,j,k') + AR(m,k')(1+f_{\nu'}) + AC(m,k')N_{\mathrm{e}}}, \tag{4}$$

$$h\nu' = E_{k'} - E_m, \tag{5}$$

where $f_{\nu'}$ represents the photon distribution function, and the sum over k' means summing over all possible k' which satisfies the autoionization energy relation

$$E_j + E_{k'} = E_m + \epsilon, \tag{6}$$

where $\epsilon \geq 0$ represents the energy of the final free electron.

Writing the branch ratio as Eq.(4), we omit the radiative transitions to non-m shell because the resonant transition to the mth shell are usually much faster than the other transitions.[14] In Eq.(4)

$$AA(m,j,k) = c_j p'_j c_k p_k (1-p'_m) A^{\mathrm{a}} \quad j \neq k, \tag{7}$$

$$AA(m,j,k) = \frac{c_j p'_j (c_j p'_j - 1)}{2} (1-p'_m) A^{\mathrm{a}} j = k, \tag{8}$$

$$AR(m,k) = c_k p_k (1-p'_m) A^{\mathrm{r}}_{mk} \qquad k \neq j, \tag{9}$$

$$AR(m,k) = c_k p'_k (1-p'_m) A^{\mathrm{r}}_{mk} \qquad k = j, \tag{10}$$

$$AC(m,k) = c_k p_k (1-p'_m) A^{\mathrm{c}}_{mk} \qquad k \neq j, \tag{11}$$

$$AC(m,k) = c_k p'_k (1-p'_m) A^{\mathrm{c}}_{mk} \qquad k = j, \tag{12}$$

where A^{a} is the auger rate for a hypothetical two-electron ion, A^{r}_{mk} and A^{c}_{mk} are the corresponding spontaneous radiative probability and collision de-excitation rate of the hypothetical one-electron ion respectively, and

$$p'_j = p_j + \delta / c_j, \tag{13}$$

$$p'_m = p_m - \delta / c_i, \tag{14}$$

$$\delta = \min(1, c_m p_m, c_j (1-p_j), c_k p_k) \qquad j \neq k, \tag{15}$$

$$\delta = \min(1.0, c_m p_m, c_k (1-p_k), c_k p_k) j = k. \tag{16}$$

III. RESULTS AND DISCUSSION

First of all, we deal with the EA rate coefficient for the average ion by DCA model. As an example we calculated the EA rate coefficient for an argon plasma using Eqs.(3)–(16). The average ion is: $c_{1\mathrm{s}}p_{1\mathrm{s}} = 2.0$, $c_{2\mathrm{s}}p_{2\mathrm{s}} = 2.0$, $c_{2\mathrm{p}}p_{2\mathrm{p}} = 3.999$, $c_{3\mathrm{s}}p_{3\mathrm{s}} = 0.05$, $c_{3\mathrm{p}}p_{3\mathrm{p}} = 0.025$. In the calculation the effect of radiative field is neglected, the electron density is $10^{20}\,\mathrm{cm}^{-3}$, the wave functions are calculated with the atom-structure program for AA model developed by Zhao *et al.*[15] The electron compact excitation cross section and the auger rate are calculated with the methods of Pindzola *et al.*[16] and McGuire[17], respectively. For comparison we also calculate the average EA rate expressed by Eq.(2) with the binomial distribution for the fractional of each configuration $N_{z,n}/N$. In addition, the EA rate coefficients from the 'real' ion(z,n) to 'real' ion$(z{+}1,m)$ are calculated by using the AA codes with integer occupation numbers. This means we use the configuration average approximation, which is much simpler than the fine structure level calculation and has a reasonable accuracy. The reasonableness to do so has been investigated by Zhao *et al.*.[15] The EA rate for the average ion and the EA rate average via DCA have been compared in Fig.1. The comparisons show that for the 2s and 2p subshell, the differences are about a factor of 1.5. Considering that the AA model is a simplified approximation, this difference is acceptable.

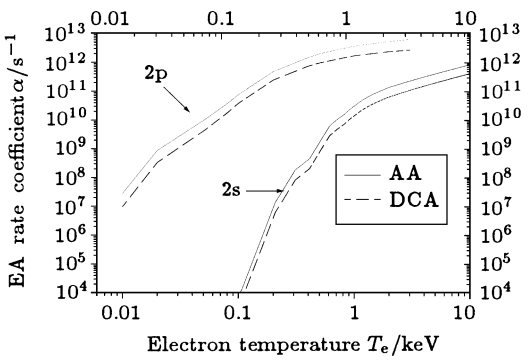


Fig.1. EA rate coefficients for the average Ar ion and the average EA rate coefficients in the 2s and 2p subshells vs electron temperature.

Now the EA process is added into the rate equations for AA model,[4,8] in which the DR process is included using Zhao's method.[15] The auger rates

used are those of He-like ions calculated by Cowan's codes.[18] In the calculation the optically thin approximation is adopted. For comparison the rate equations without EA are also solved.

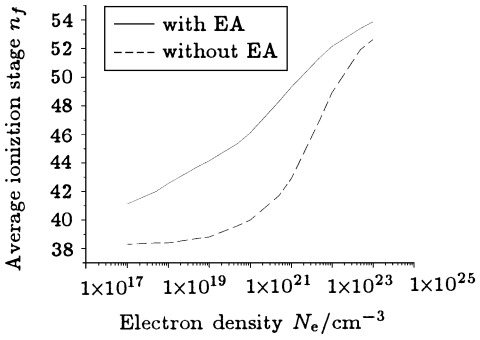


Fig.2. The average ionization stage n_f of Lu plasmas vs electron density. The solid line is the result with EA and the dashed line without EA.

Figure 2 shows the average ionization stage n_f of Lu plasma varying with electron density N_e, the electron temperature is fixed at 1.6 keV. The solid curve represents the results of that including EA and the dashed curve the results without EA. The comparison shows that the EA effect is significant usually at low electron density and weakens at high electron density and the two curves are expected to reach each other if N_e is so large that the plasma is approximately at LTE condition. This could explain the fact that although the electron compact excitation rate is proportional to N_e, the branch ratio becomes smaller when N_e increases since the de-excitation branch increases with N_e while the auger rate does not change with it. The competition of the two opposite trends with N_e determines the variation of EA effects. The additional ionization caused by EA is less than 10% for N_e ranging from 10^{18} to 10^{19} and reaches its maximum value of about 15% for N_e from 10^{21} to 10^{22} cm^{-3}.

Figure 3 shows the average ionization stage n_f of Au plasma versus electron temperature, the electron density being fixed at 10^{20} cm^{-3}. The solid curve is the results including EA and the dashed one is those without EA. From the comparison in Fig.3, we can see that generally speaking, the EA effect is not so large at low temperatures but becomes stronger at high temperatures. The EA process creates an additional ionization of the maximum value 15% or so at $T_e = 2.0$ keV.

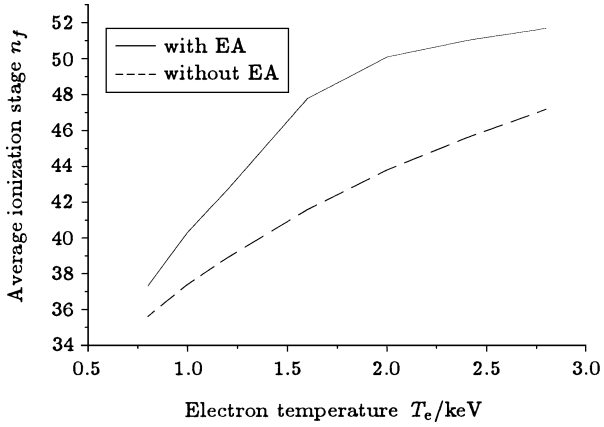


Fig.3. The average ionization stage n_f of Au plasmas vs electron Temperature. The solid line is the result with EA and the dashed line without EA. Au, $N_e = 10^{20}$ cm^{-3}.

IV.CONCLUSION

We have proposed a method to calculate EA rate for average ions and solved the AA rate equations for investigating the EA effect. Although the numerical example shows some difference between the EA rate for average ion and the average EA rate, this discrepency is acceptable for the aim of AA model. The numerical results of average ionization state indicate when and how much the EA process influences the electron distribution. We could conclude that the range in which the EA effect appears strong is just similar to that of the DR process, i.e., the high-temperature low-density range. As we know, the DR can considerably decrease the ionization stage in high-temperature low-density plasmas (especially for high-Z plasmas), hence it is neccessary to include EA process in the same range; otherwise, the DR effect may be overestimated up to 15%, as indicated by the present data. We expect that accounting for the EA process in the non-LTE models may improve the accuracy in predicting electron distribution.

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