Enhancement of the excitation and deexcitation rate coefficients of ions in dense plasmas: The role of autoionizing states

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(Received 2 January 1985)

In processes of excitation—deexcitation and of ionization—recombination of ions immersed in dense plasmas, multistep processes through various intermediate states are important. In the present paper we deal with the excitation and deexcitation that have doubly excited, or autoionizing, states as intermediate states. We call these the dielectronic-capture ladderlike (DL) processes. Hydrogenlike $1s\leftrightarrow 2s$ or $1s\leftrightarrow 2p$ transitions are considered for the purpose of illustration. The DL excitation rate coefficient is obtained as a function of electron density with an approximation that is based on the picture of dielectronic capture of the $1s$ ion into the doubly excited states followed by the collisional ladderlike excitation-ionization chain. The DL deexcitation rate coefficient results from autoionization of the doubly excited level ions that are in local thermal equilibrium with respect to the $2l$-level populations (l is s or p). Both of the rate coefficients are interpreted as an extrapolation of the excitation cross section due to lowering of the threshold energy of the $1s\rightarrow 2l$ excitation and are found to obey the principle of detailed balance. Thus, the DL processes may be regarded as enhancements of the direct excitation and deexcitation. A detailed collisional-radiative-model calculation, which includes 60 doubly excited levels and relevant collisional and radiative transitions, is performed, and the above approximations are found to be consistent with the results.

I. INTRODUCTION

Properties of atoms and ions immersed in a dense plasma have been studied recently in relation to the inertial confinement fusion research. For example, the effects of dense surroundings on the atomic transition oscillator strength[1–4] and on the excitation cross section of ions[5,6] have been calculated by using various approximations; these quantities tend to decrease with an increase in the plasma density owing to the Debye screening. Density effects on the excitation and deexcitation rate coefficients that are due to multistep processes via various intermediate states draw little attention. Fujimoto and Kato[7] proposed a new excitation process, i.e., the dielectronic-capture ladderlike (DL) excitation involving autoionizing states as intermediate states. In the present paper we present a detailed calculation on the DL excitation and deexcitation processes. Section II gives an approximate treatment of the problem; this will give readers insight into the physical picture of the processes. A detailed numerical calculation follows. Finally, discussion on the validity range and other relevant parameters is given.

II. DL EXCITATION AND DEEXCITATION: APPROXIMATION

We consider as an example the DL processes in a hydrogenic ion.

A. Excitation

We consider the excitation process of $1\rightarrow p$, where 1 denotes the ground state $1s$. Figure 1 depicts a schematic energy-level diagram relevant to the processes concerned. Associated with the excited level p we have a series of doubly excited levels (heliumlike) pq, where q denotes the state of the outer electron and p denotes the state of the core electron. Upon collisions with electrons, the ground-state ion 1 may undergo dielectronic capture into state pq. Let its rate coefficient be denoted by $r_d(pq)$. The doubly excited ion thus produced may autoionize, $pq\rightarrow 1+e$ [with probability $A_a(pq)$], where e denotes the electron in a continuum state, or make a radiative transition, $pq\rightarrow pq'+h\nu'$ [$q'<q$, with probability $A_r(pq,pq')$; here q and q' are understood to denote the principal quantum number of the states concerned], or make a stabilizing transition $pq\rightarrow 1q+h\nu$ [$A_r(pq,1q)$]. The last process is dielectronic recombination. However, when the electron density n_e is high, collisional processes may become important on the ion state pq. For example, this ion may be excited, $pq+e\rightarrow p(q+1)+e$ (with collisional rate coefficient $C[pq,p(q+1)]$), before it autoionizes or decays radiatively. The latter ion undergoes further excitation $p(q+1)\rightarrow p(q+2)\rightarrow\cdots\rightarrow pr$ ($r\gg q$), and finally it is "ionized,"[8] $pr+e\rightarrow p+2e$, to leave a hydrogenlike ion p. This series of processes, called dielectronic-capture ladderlike excitation[7] is, in effect, the excitation of the hydrogenic ion, $1+e\rightarrow p+e$. In evaluating the excitation rate coefficient of ions in a plasma, this contribution

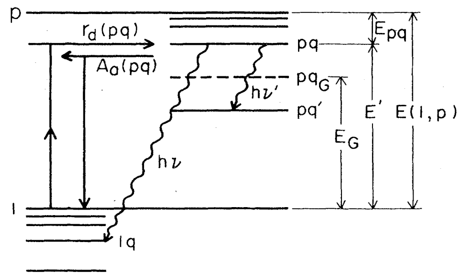

FIG. 1. Schematic energy-level diagram relevant to the DL excitation and deexcitation processes.

should be included besides the direct excitation.

It is well known for singly excited hydrogenlike ions q that the radiative decay rate decreases with an increase in q, roughly in proportion to $q^{-4.5}$, while the depopulation rate by electron collisions, the main part of which is the excitation to the adjacent-lying higher level, increases in proportion to q^4. Then, for a given n_e we can define the critical level q_G for which the radiative and collisional depopulation rates are equal.[9] For the levels lying below this, the population decays downward by radiative transitions, while for the levels lying above that, the population is lost by electronic collisions, predominantly by excitation to the higher-lying levels. We call this critical level Griem's limit or the collision limit.[8–11]

For doubly excited ions we define a similar collision limit pq_G such that the depopulating electron collision rate is equal to the sum of the autoionization probability and the radiative transition probabilities,

$$A_a(pq)+\sum_{q'\,(<q)} A_r(pq,pq')+A_r(pq,1q) .$$

Then, we may assume that electrons dielectronically captured into the states lying below pq_G are lost by autoionization or by radiative decay, but that electrons captured into the levels higher than pq_G are further excited, and finally undergo the DL excitation process. On the basis of the above picture we may estimate the magnitude of the rate coefficient for the DL process.

Let the DL excitation rate coefficient be denoted by $C_{\rm DL}(1,p)$. Then, the rate per unit volume of the DL excitation process in the plasma is expressed as

$$C_{\rm DL}(1,p)n(1)n_e \simeq \sum_{q\,(\geq q_G)} n(1)r_d(pq)n_e \ , \tag{1}$$

where $n(p)$ stands for the population density of the hydrogenlike ion in state p. The DL excitation rate coefficient is given as

$$C_{\rm DL}(1,p)\simeq \sum_{q\,(\geq q_G)} r_d(pq) \ ,$$

and this may be approximated for a large q_G as

$$C_{\rm DL}(1,p)\simeq \int_{q_G}^{\infty} r_d(pq)dq \ . \tag{2}$$

The quantum-defect theory shows that the dielectronic-capture rate coefficient may be expressed as an extrapolation of the excitation cross section $\sigma(1,p)$ below the excitation threshold,

$$r_d(pq)=f(E')v\sigma(1,p)\frac{dE'}{dq} \ , \tag{3}$$

where $f(E')$ is the electron energy distribution function at E', the energy of the captured electron, and v is its velocity. We change the integration variable from q to the electron energy. Then, we arrive at

$$C_{\rm DL}(1,p)\simeq \int_{E_G}^{E(1,p)} f(E')v\sigma(1,p)dE' \ , \tag{4}$$

where E_G is the energy of the critical level as measured from the ground state, and $E(1,p)$ is the threshold energy for the direct excitation $1\rightarrow p$ (see Fig. 1). In the above we have used the relation

$$dE'=\frac{2(z-1)^2R}{q^3}dq \ , \tag{5}$$

where R is one rydberg (13.6 eV) and z is the nuclear charge.

Equation (1) or (4) corresponds to the approximation that the electrons dielectronically captured into the doubly excited states above the collision limit neither autoionize nor undergo dielectronic recombination. Rather, they are "ionized" and enhance the excitation $1\rightarrow p$. Thus, as shown in Fig. 2, the DL excitation may be understood as the lowering of the threshold energy of the direct excitation, $E(1,p)$, to the energy of the critical level, E_G.

The critical level is defined by

$$\sum_{q'\,(>q)} C(pq,pq')n_e = A_a(pq)+\sum_{q'\,(<q)} A_r(pq,pq') + A_r(pq,1q) \ . \tag{6}$$

In the collision term we retain only the dominant collision rate coefficient $C(pq,p(q+1))$ as a rough approximation and approximate it by a formula for a normal hydrogenic ion[9,12]

$$C(q,q+1)=\frac{8.69\times10^{-8}}{(z-1)^3}\left[\frac{(z-1)^2R}{kT_e}\right]^{1/2} \times\frac{(z-1)^2R}{E_{q,q+1}}f_{q,q+1}\ {\rm cm^3\,s^{-1}} \ , \tag{7}$$

where $E_{q,q+1}$ and $f_{q,q+1}$ stand for, respectively, the energy difference and the oscillator strength between the levels q and $q+1$. $f_{q,q+1}$ is approximated to $q/2^2$,[8] and $E_{q,q+1}$ is written as $2(z-1)^2R/q^3$. For $\sum_{q'\,(<q)}A_r(pq,pq')$ we take $(z-1)^4 1.65\times10^{10}q^{-4.5}\ {\rm s^{-1}}$, and $A_r(pq,1q)$ is given

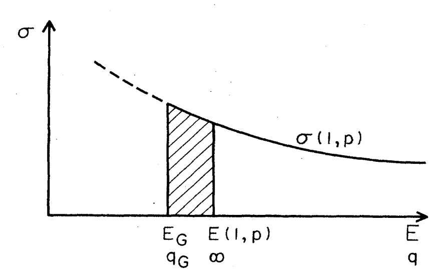

FIG. 2. Interpretation of the DL processes as an extrapolation of the excitation cross section below the excitation threshold down to Griem's limit.

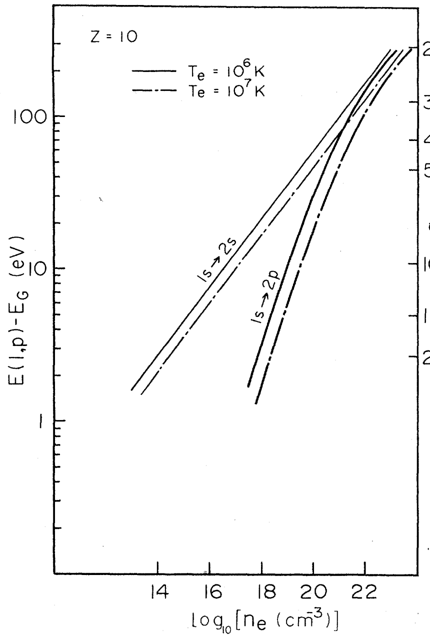

FIG. 3. Examples of the estimated Griem's limit for the doubly excited heliumlike neon ion. The lowering of the energy from the original excitation threshold is given as a function of the electron density.

from the corresponding hydrogenlike transition $A_r(p,1)$. A_a is given as the inverse process to Eq. (3),

$$A_a=\frac{4(z-1)^2E'}{hq^3}\frac{g(1)}{g(pq)}\frac{\sigma(1,p)}{\pi a_0^2}\ , \tag{8}$$

where $g(p)$ denotes the statistical weight and a_0 is the first Bohr radius.

We take as examples the excitation process of hydrogenlike ion $1s\rightarrow 2s$ and $1s\rightarrow 2p$. For the direct-excitation cross section $1s\rightarrow 2s$ and $2p$, we take the cross sections based on the close-coupling calculations:[13,14] the collision strength is given by $z^2\Omega=0.9345-1.125/x+1.410/x^2-0.4620/x^3$ for $1s$-$2s$, where x denotes the energy in the threshold units, and $z^2\Omega=-5.341+10.12/x-1.807/x^2+7.020\ln x$ for $1s$-$2p$. Figure 3 gives the critical level obtained from Eq. (6) for the case of a neon ion: Fig. 3 gives the energy $E(1,2)-E_G$ as a function of n_e. The upper end of the lines corresponds to $q_G=2$.

By using Eq. (4) we calculate the rate coefficients. Figures 4(a) and 4(b) show the results for temperatures of 10^6 and 10^7 K, respectively, for the case of a neon ion. In Fig. 4 the rate coefficients for the direct excitation are shown by the horizontal bars. The total excitation rate coefficient is given as a sum of these two components. The DL contribution is substantial for the low-temperature case.

Figures 5 and 6 give a few other examples. The temperature corresponds approximately to the optimum temperature at which the emission lines have their maximum intensities under the corona equilibrium condition.

B. Deexcitation

We assume the recombining plasma situation[11] in which we have zero population in the ground state. The

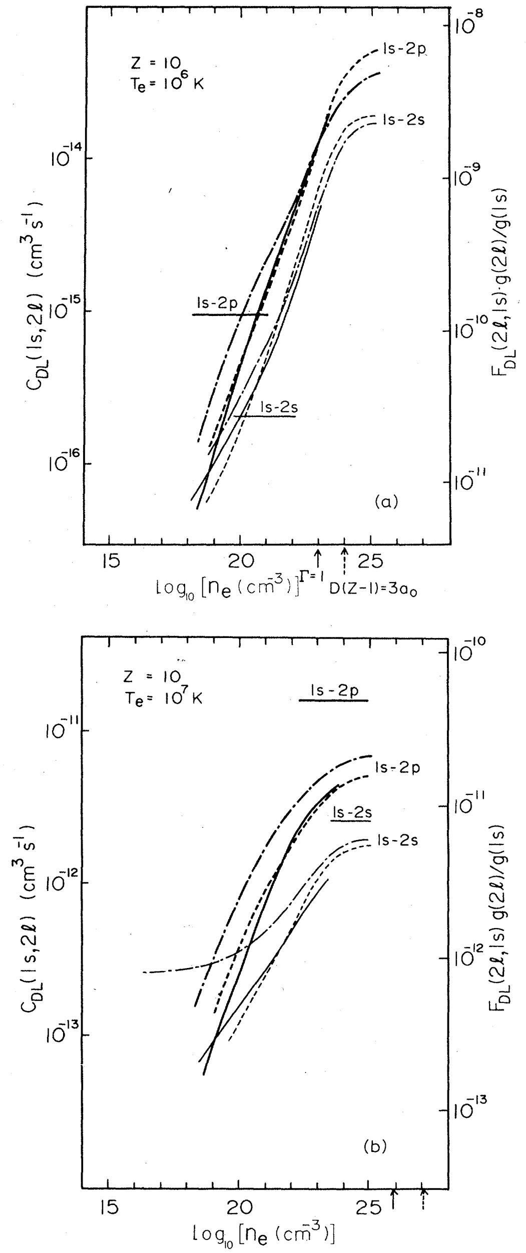

FIG. 4. DL excitation and deexcitation rate coefficients for hydrogenlike neon-ion transitions $1s$-$2s$ (thin curves) and $1s$-$2p$ (thick curves). ——, approximation [Eq. (4) or Eq. (14)]. - - - -, numerical calculation for $C_{\rm DL}(1s,2l)$. — — —, numerical calculation for $F_{\rm DL}(2l,1s)$, the right-hand-side ordinate is applied. Dashed arrow shows n_e at which the lowering of the ionization potential reaches to $n'=2$ level, and the solid arrow shows n_e at which $\Gamma=1$. (a) Temperature is 1.0×10^6 K. (b) Temperature is 1.0×10^7 K.

heliumlike ion in level pq that is produced by "recombination" of a hydrogenlike ion p may undergo autoionization. This process is, in effect, the deexcitation of $p+e\rightarrow 1+e$. In terms of the collisional-radiative model the population density of the heliumlike ion pq is given by the population density of the hydrogenlike ion p, under our assumption

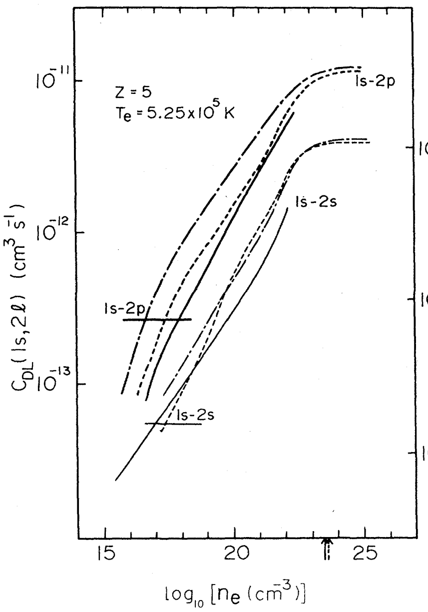

FIG. 5. DL excitation and deexcitation rate coefficients for hydrogenlike boron-ion transitions. $T_e = 5.25 \times 10^5$ K. Explanation same as for Fig. 4.

$$n(pq) = r_0(pq)Z(pq)n(p)n_e \;, \tag{9}$$

where $r_0(pq)$ is the population coefficient and $Z(pq)$ is the Saha-Boltzmann coefficient

$$Z(pq) = \frac{g(pq)}{2g(p)} \left[\frac{h^2}{2\pi mkT_e} \right]^{3/2} \exp(E_{pq}/kT_e) \;, \tag{10}$$

where E_{pq} is the "ionization" potential of level pq (see

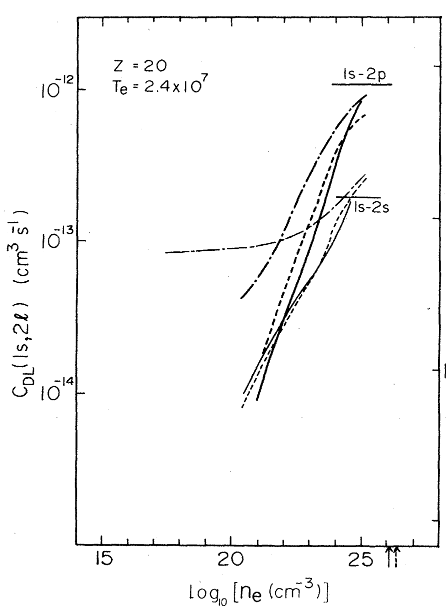

FIG. 6. DL excitation and deexcitation rate coefficients for hydrogenlike calcium-ion transitions. $T_e = 2.4 \times 10^7$ K. Explanation same as for Fig. 4.

Fig. 1) and other symbols have their usual meanings. The rate per unit volume of deexcitation by this process is expressed as

$$F_{\mathrm{DL}}(p,1)n(p)n_e = \sum_q n(pq)A_a(pq)$$
$$= \sum_q r_0(pq)Z(pq)n(p)n_e A_a(pq) \;, \tag{11}$$

where $F_{\mathrm{DL}}(p,1)$ is the DL deexcitation rate coefficient, and it is given by

$$F_{\mathrm{DL}}(p,1) = \sum_q r_0(pq)Z(pq)A_a(pq) \;. \tag{12}$$

It has been shown[11] for singly excited ions that the levels q lying above the collision limit have the population coefficient $r_0(q) \simeq 1$ unless the temperature is very low, and the lower levels have $r_0(q) \ll 1$. The similar situation is expected for the doubly excited levels. Thus we set

$$r_0(pq) = \begin{cases} 1 & \text{for } q \geq q_G \\ 0 & \text{for } q < q_G \;, \end{cases} \tag{13}$$

then we have

$$F_{\mathrm{DL}}(p,1) \simeq \sum_{q\,(\geq q_G)} Z(pq)A_a(pq) \;. \tag{12$'$}$$

By using Eqs. (8) and (10) and the Maxwellian distribution for $f(E')$ we obtain

$$F_{\mathrm{DL}}(p,1) \simeq \frac{g(1)}{g(p)} \exp[E(1,p)/kT_e]$$
$$\times \int_{E_G}^{E(1,p)} f(E')v\sigma(1,p)dE' \;. \tag{14}$$

It should be noted that the DL excitation rate coefficient $C_{\mathrm{DL}}(1,p)$ and the DL deexcitation rate coefficient $F_{\mathrm{DL}}(p,1)$ obey the principle of detailed balance, Eqs. (4) and (14). The excitation energy, however, is not E_G but the original threshold energy $E(1,p)$. Thus, the result of the approximate calculation for $F_{\mathrm{DL}}(p,1)$ is identical to that of $C_{\mathrm{DL}}(1,p)$, as given by the solid curve in Figs. 4–6.

III. NUMERICAL CALCULATION

The system of the doubly excited states $2ln'l'\,^{2S+1}L$ is considered with 60 levels of $2 \leq n' \leq 20$, and the rate coefficients for the collisional and radiative transitions between these levels are approximated by those of the heliumlike ion states $1sn'l'\,^{2S+1}L$.[15] These processes are the following.

(1) Excitation-deexcitation: $2ln'l' + e \leftrightarrow 2ln''l'' + e$. We primarily rely on the infinite-z hydrogenic approximation by Sampson and Parks.[16] Small modifications which have been made for the normal heliumlike ions[15] are kept in the present calculation.

(2) Radiative transition: $2ln'l' \rightarrow 2ln''l'' + h\nu'$. For optically allowed transitions the absorption oscillator strength is given by

$$f = f_{\mathrm{H}} - \Delta f/(z-1) \;, \tag{15}$$

where f_{H} stands for the hydrogenic value and Δf has been determined for the case of normal heliumlike ions.

(3) Ionization and three-body recombination: $2ln'l' + e \leftrightarrow 2l + 2e$. In this case the "ion" is the excited $2l$-state ion. The empirical formula by Lotz[17] is adopted.

(4) Radiative recombination: $2l + e \rightarrow 2ln'l' + h\nu''$. For the photoionization cross section the hydrogenlike values are employed.

Since the levels considered above are doubly excited states, transitions connecting these levels to the ground-state hydrogenlike level and to the normal heliumlike levels are included.

(5) Dielectronic capture and autoionization: $1s + e \leftrightarrow 2ln'l'$. For the levels $n' \geq 3$ the dielectronic-capture rate coefficient or the autoionization probability is calculated from the direct and exchange reactance matrix elements[18] for the excitation cross section of the hydrogenic $1s$-$2l$ transition. For $2l2l'$ the autoionization probability is estimated from Ref. 19.

(6) Stabilizing radiative transition: $2pn'l' \rightarrow 1sn'l' + h\nu$. The transition probability for the hydrogenic $2p \rightarrow 1s$ transition is adopted.

(7) Stabilizing collisional transtion: $2ln'l' + e \rightarrow 1sn'l' + e$. The deexcitation rate coefficient for the hydrogenic $2l \rightarrow 1s$ transition[13,14] is adopted.

The system of the coupled collisional-radiative equations[15,20] are constructed for $1s$, $2ln'l'$, and $2l$, where l is s or p. The above rate coefficients and transition probabilities are used, and the method of the quasi-steady-state solution is applied. The effective excitation rate coefficient $1s \rightarrow 2l$ which consists of the processes through intermediate doubly excited states are obtained as the DL excitation rate coefficient $C_{\rm DL}(1s,2l)$, and the DL deexcitation rate coefficient $F_{\rm DL}(2l,1s)$ is obtained similarly. In order to avoid counting the $2s2p$ state twice as a $2s$ core state and a $2p$ core state, an appropriate correction has been made. Examples of the results are shown in Figs. 4—6.

IV. DISCUSSION

The agreement between the numerical calculation in Sec. III and the approximation in Sec. II is reasonably good. The principle of detailed balance is not obeyed by the numerically obtained $C_{\rm DL}(1s,2l)$ and $F_{\rm DL}(2l,1s)$; this is because the approximations (1) and (12′) are not strictly valid.

One interesting feature is seen for higher temperatures. In Fig. 6, for example, the DL deexcitation rate coefficient has a finite value for small electron densities. This is understood from the fact that, for the case of normal hydrogenlike levels, the balance between the radiative recombination and the radiative decay (this balance is called the capture-cascade scheme[21]) leads to the population density approximately equal to the LTE (local thermodynamic equilibrium) value[22] or $r_0(q) \simeq 1$ even if q were smaller than q_G. In our present case the autoionization and the stabilizing transitions are added to the radiative decay, but the essential feature remains unchanged. Thus the approximation of Eq. (13), $r_0(pq) = 0$ for $q < q_G$, is not correct for the high temperatures: $r_0(2ln'l')$ has a value of the order of unity instead of 0 for the low-density regions. Thus in Eq. (12′) lower-lying levels than p_G should be taken into account. This leads to the finite contribution from the DL deexcitation.

In our calculation the doubly excited levels as high as $n' = 20$ are calculated, and the levels $21 \leq n' \leq 25$ are assumed to be in LTE, i.e., $r_1(2ln'l') = 0$ and $r_0(2ln'l') = 1$. Under the condition of high electron densities, "the lowering of the ionization potential" occurs. It might be claimed that under such conditions the calculation including such high-lying levels as $n' = 20$ would lead to an error. However, this is not the case. The reason is as follows: It is well known in the quantum-defect theory that many atomic parameters for discrete levels continue smoothly across the ionization limit to the continuum states. For instance, the Gaunt factor for the oscillator strength of series lines continues smoothly to the Gaunt factor of the photoionization cross section. Furthermore, this continuation property as well as the absolute magnitude of the oscillator strength do not change much with an increase in the density, say, until the Debye length becomes 10 times the radius of the $1s$-electron orbit.[4] On the other hand, with an increase in the electron density the high-lying levels enter either into LTE for a recombining plasma or into the ladderlike excitation-ionization chain for an ionizing plasma;[11,8] in both cases these levels are strongly coupled with the continuum states. The lower end of these "quasicontinuum" states is given by Griem's criterion, Eq. (6) in the present case, and the "lowering" occurs at much higher levels. Thus, even if the latter phenomena takes place, unless the electron density is so high that the low-lying levels such as $n' = 2$ are strongly affected, both treatments, in which the high-lying levels are considered as discrete or continuum, make little difference. In Figs. 4—6 the density at which the "lowering" reaches $n' = 2$ levels[23] is indicated with a dashed arrow.

A few calculations[5,6] have been reported on the density dependence of the excitation cross section. In the approximations employed it decreases with an increase in the density owing to the Debye screening. Thus this decrease tends to cancel the increase in the excitation and deexcitation rate coefficients as given above.

Jacobs and Davis[24] present an extensive calculation of ion populations and ionization-recombination rates, including many levels and processes which may become important when the plasma density is high. However, they neglect ionization from and recombination to the doubly excited levels: these are the important processes as discussed in the present paper. Another example of the manifestation of these processes is that the resonance contribution to the excitation cross section is diminished in a dense plasma: the resonance excitation process, e.g., $1s + e \rightarrow 3lnl' \rightarrow 2l'' + e$, in a low-density plasma is taken over in the dense plasma by the DL excitation process, $1s + e \rightarrow 3lnl' + (e) \rightarrow 3l(n+1)l'' + (e) \rightarrow \cdots \rightarrow 3l + e$.

Another multistep excitation process which might be important but is neglected in the present investigation is recombination from $1s$ to the high-lying heliumlike ion followed by ionization to the hydrogenlike excited levels. The corresponding rate is found to give an insignificant contribution to the effective excitation rate: a rough estimate shows that its contribution does not exceed 1% of the DL excitation rate coefficient under the condition of

Fig. 4(a).

The present treatment breaks down when the coupling parameter Γ becomes of the order of unity. Under the condition that the ions concerned are immersed in a hydrogen plasma as an impurity the parameter is given by

$$\Gamma=\frac{(z-2)e^2}{kT_e}\left[\frac{4\pi n_e}{3}\right]^{1/3} . \tag{16}$$

In Figs. 4—6 the electron density at which $\Gamma=1$ holds is given with the solid arrow.

ACKNOWLEDGMENTS

The authors are grateful to Dr. P. Kunasz for a critical reading of the manuscript.

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