Ionization and recombination rates in non-Maxwellian plasmas

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The ionization, excitation, and radiative recombination rates for highly stripped ions are calculated with Maxwellian and non-Maxwellian electron distribution functions of the type $C_m \exp(-v^m/w^m)$ $(2 \le m \le 5)$ as encountered in laser-heated plasmas and certain types of turbulent plasmas. The direct-radiative-recombination rates are found to decrease by at most 30% as *m* is increased from 2 to 5. On the other hand, the ionization and excitation rates are found to be strongly reduced if the transition energy χ exceeds twice the local temperature $k_B T_e$. The effect of this on the distribution of energy levels and degrees of ionization in laser-produced plasmas could be important.

Electron distribution functions in laser-heated plasmas can be strongly non-Maxwellian. In this Brief Report, we will show how this affects the rates of ionization, recombination, and excitation. In the first part of the paper, we give a simple formula for the electron distribution function in the underdense (i.e., of density below the critical density) part of a plasma heated by classical absorption of laser light. In the second part, we use these electron distribution functions to compute the rates of ionization, recombination, and excitation and compare these rates to the usual ones which are obtained by assuming a thermal (Maxwellian) electron distribution function with the same density and temperature.

Electron distribution functions of the type

$$f_m(v) = C_m \exp(-v^m / V_m^m) , \qquad (1a)$$

where

$$C_m = m / [\Gamma(3/m)V_m^3], \qquad (1b)$$

$$V_m^2 = (k_B T_e / M_e) [3\Gamma(3/m) / \Gamma(5/m)], \qquad (1c)$$

occur in several plasma-physics situations. For m=2, (1) is the usual Maxwell-Boltzmann distribution function. In turbulent plasmas (e.g., in the presence of ion-acoustic turbulence), Dum¹ has shown that values of m=3.6 to 4 or even 5 could be obtained. Also, Langdon² has shown that in laser-produced plasmas, inverse bremsstrahlung (IB) heating produces a distribution function with m=5, if electron-electron (e - e) collisions are neglected. Langdon also exhibited distributions for the case where e - ecollisions compete with IB, but did not characterize these in terms of (1), except to show the reduction of f(v) at the origin, which causes reduced absorption of the laser flux.

Numerical simulations of laser-plasma interaction have recently been performed with Fokker-Planck codes by Albritton³ and by Matte *et al.*⁴ which included IB, e - e, and electron-ion (e-i) collisions, transport, and, in Ref. 4, ion motion. These showed non-Maxwellian distribution functions occurring in the underdense plasma for the conditions that were studied $(ZI\lambda^2 \ge 10^{15} \text{ W} \mu \text{m}^2/\text{cm}^2)$. Later on, Matte *et al.*^{5,6} and Lamoureux⁷ analyzed the results of the FPI (Fokker-Planck International) Fokker-Planck code⁴ including e - e collisions and IB heating, and studied the resulting radiative recombination and bremsstrahlung spectra. They demonstrated the distribution functions in the underdense plasma to be well represented by formula (1) with the value of *m* depending on the Langdon parameter²

$$\alpha = Z v_{\rm osc}^2 / v_{\rm th}^2 = \frac{42Z}{k_B T \ (eV)} \frac{I \lambda^2}{10^{14} \ W \ cm^{-2}} \\ \times \frac{(1 - N_e / N_c)^{1/2}}{(1.06 \ \mu m)^2} \ .$$
(2)

A good fit (a few percent) for the relation $m(\alpha)$ is^{6,7}

$$m(\alpha) = 2 + 3/(1 + 1.66/\alpha^{0.724}).$$
(3)

In formula (2), Z is the average atomic number, $v_{\rm osc}$ is the oscillation velocity of an electron in the laser electric field, I is the laser intensity in W/cm², $k_B T$ is the electron temperature in eV, λ is the vacuum wavelength in micrometers, N_e is the electron density, and N_c is the critical density. The laser intensity I to be used in (2) is not necessarily the incident intensity I_0 , but rather the intensity at the position considered (including the reflected beam and considering the absorption below and above N_e).

For example, if we apply the above formulas to our own Fokker-Planck simulation⁴ $(I_0=3\times10^{14} \text{ W/cm}^2, \lambda_0=1.06 \ \mu\text{m}, Z=4, T=2.3 \text{ keV})$ we have, at $N_e=N_c/4$, negligible absorption below N_e and 37% absorption above. Thus, $I=1.63I_0$ and we obtain $\alpha=0.41$ and m=2.72. In high-Z plasmas, this effect can be even stronger. For example, if $I=4\times10^{14}$ W/cm², $\lambda=0.53$ μ m, $kT_e=1000$ eV, and Z=50, we have m=3.52.

The corresponding analysis (and therefore the values for m) must be reconsidered in the immediate vicinity of the critical surface, where α becomes large due to the swelling factor $(1 - N_e/N_c)^{-1/2}$ for density slightly below critical and is zero for densities above critical. It is then found⁶ that the slow electron distribution is in near agreement with the local high value for α , while the fastest electron distribution is closer to Maxwellian because of the proximity of the overdense region. As an illustration, if we consider again the conditions of Ref. 4 as listed above, we obtain m=3.0 for slow and m=2.6 for fast electrons at $N_e=0.9N_c$.

The presence of f_m -type distributions [Eq. (1)] in laserproduced plasmas and in other important cases has prompted us to study the effect of the shape of the distribution function (as characterized by the value of m) on the rates of ionization, excitation, and direct-radiative recombination. These rates determine the populations of the various ionization degrees and energy levels in the plasma, hence the necessity of knowing them accurately. To date, plasma simulation codes which include ionization and recombination effects assume a Maxwellian electron distribution to calculate the rates.⁸

The rates are obtained by integration of the cross section over the distribution function. For ionization and recombination, we have, respectively,

$$S_{c} = \langle \sigma_{I}(v)v \rangle = 4\pi \int_{0}^{\infty} \sigma_{I}(v)v^{3}f(v)dv , \qquad (4)$$

$$\alpha_R = \langle \sigma_R(v)v \rangle = 4\pi \int_0^\infty \sigma_R(v)v^3 f(v) dv .$$
 (5)

A good estimate of the effects of the distribution function on ionization rates can be obtained using the simple Lotz formula⁹

$$\sigma_I = (0.7)4\pi a_0^2 \left[\frac{\chi_H}{\chi}\right]^2 \xi \frac{\ln(E/\chi)}{E/\chi} \quad (E \ge \chi) , \qquad (6)$$

where $E = \frac{1}{2}M_ev^2$ is the kinetic energy of the incident electron, χ is the ionization potential of the ion, a_0 is the Bohr radius, χ_H is the ionization potential of hydrogen (13.6 eV), and ξ is the number of electrons to be ionized, which we will assume to be 1 in our case.

In a similar way, the main features of the directradiative-recombination cross section for level n are well reproduced by the hydrogenic cross section¹⁰

$$\sigma_R = \frac{32\pi}{3\sqrt{3}} \alpha^3 a_0^2 \frac{n}{(E/\chi)(1 + E/\chi)} , \qquad (7)$$

where α is the fine-structure constant [not to be confused with the α defined in Eq. (2)]. We have assumed recombination to the ground level (n=1) for simplicity in our calculations.

We have used these cross sections to calculate the collisional ionization and radiative-recombination rates between the ground states of two adjacent ionic species for several values of m in (1) (m=2, 3, 4, and 5) and for a given value of the ionization potential χ . In Fig. 1, we give the rates as a function of temperature for $\chi=2000$ eV. This value of χ is appropriate for He-like or H-like aluminum, or for *M*-shell gold ions. As is readily seen, the effect on recombination is rather modest: a 20-30% reduction of the rates for m=5 compared to m=2. The reason for this reduction is the lower number of slow electrons,² for which the recombination cross section is larger. For the same reason, such non-Maxwellian distributions lead to a modest reduction of the total power loss for this process.¹¹

On the other hand, a very important reduction of the ionization rate is seen as m increases, particularly if the temperature is low: between m=2 and 5, the decrease is two orders of magnitude at T = 400 eV, 1 order of magnitude at T=600 eV, and approximately 30% at 1 keV. The values of the cross sections [Eqs. (6) and (7)] are in fact dependent on the ratio E/χ of the incident electron energy to the energy of the transition considered. As a consequence, the ratio $S_c(m)/S_c(MB)$ of the ionization rate calculated for a distribution (1) with parameter m to the Maxwell-Boltzmann distribution value (MB: m=2) turns out to depend only on the ratio χ/k_BT for a given value of m. Accordingly, we have plotted this ratio $S_c(m)/S_c(MB)$ as a function of $\chi/k_B T$ for several values of m in Fig. 2(a) and with a logarithmic scale in Fig. 2(b) to better illustrate the behavior for high values of χ/k_BT . It is observed that the ionization rate for a distribution with parameter $m \ge 2$ is slightly higher (20%) for $\chi/k_BT \simeq 1$, and significantly reduced (40-80% for m=3-5) for $\chi/k_BT \simeq 3$. For even higher values $\chi/k_BT \simeq 5$, the calculated rate may be one to three orders of magnitude lower in the range m = 3-5. Since this reduction is only dependent on χ/k_BT , we believe these curves may be used to correct ionization rates for atomic physics simulations in the underdense plasma with estimates for m being given by (2) and (3). The reduction of



FIG. 1. Collisional ionization (S_c) and direct-radiativerecombination (α_r) rates vs temperature T_e (eV) for Maxwell-Boltzmann (MB: m=2) and non-Maxwellian (m=3, 4, and 5) electron distributions of type f_m [Eq. (1)], for an ionization potential $\chi = 2000$ eV.



FIG. 2. Ratio of the collisional-ionization rate for non-Maxwellian (m=3, 4, and 5) electron distribution functions f_m [Eq. (1)] to that for a Maxwellian f_2 distribution (MB: m=2): $S_c(m)/S_c(2)$ vs the ratio of the ionization potential to the temperature χ/k_BT . Only the scales differ between (a) and (b).

the ionization rates is due to the strong reduction in the number of electrons with energy $\geq \chi$, when m > 2 and $\chi \geq 3k_B T$.

We have carried out similar calculations for collisional excitation (bound-bound) transitions. A good description of the corresponding cross sections in a general case can be obtained using Mewe's formula:¹²

$$\sigma_{ij} = 4\Pi a_0^2 \frac{2\Pi}{\sqrt{3}} \left[\frac{\chi_H}{\chi_{ij}} \right]^2 f_{ij} \frac{g(E/\chi)}{E/\chi}$$
(8)

with

$$g(U) = A + BU^{-1} + CU^{-2} + D \ln U \quad (U \ge 1) ,$$

where χ_{ij} is the excitation energy for transition between levels *i* and *j* and f_{ij} is the corresponding oscillator strength. Coefficients for g(U), the Gaunt factor approximation, are listed by Mewe in his article for several kinds of transitions. For optically allowed lines, the logarithmic term is strongly dominant, and σ_{ij} has the same asymptotic dependence as Lotz's formula (6). Therefore, the correction to the rates as a function of χ_{ij}/k_BT is well represented by Figs. 2(a) and 2(b) for a given *m*. On the other hand, for optically forbidden lines, D=0 and the corresponding excitation rate is slightly less dependent on the value of m (for example, the ratio of the m=4 to m=2 rates at $\chi_{ij}/k_B T_e = 10$ is 4×10^{-7} instead of 10^{-7}).

It should be pointed out that the calculations of distribution functions referred to above which led to the f_m form (1) were carried out for a fully ionized plasma. In applying the formulas (2) and (3) to determine the value of m, we then assume that the ionization process does not significantly modify the shape of the distribution function itself. Preliminary results from work presently in progress in our group to study the influence of atomic physics on thermal transport properties seem to confirm this point, at least in conditions typical to those encountered in coronal plasmas.

Another important point is to determine whether the cross sections that were used are a good approximation for actual atomic species encountered in laser plasmas. Indeed, the cross sections (6) and (7) are accurate within a factor of 2 (Ref. 13) in most cases. Furthermore, the uncertainty is mostly on the value of the numerical coefficients; the energy dependence of the cross sections should be much more accurate, especially in the high-energy limit. The degree of confidence in the values of ratios obtained in Figs. 2(a) and 2(b) should then be quite high, because the electrons responsible for most of the effect are in the high-energy range.

The influence of this modification of the rates on ionic and excited level populations remains to be investigated. Under coronal equilibrium conditions, the ratio of adjacent ionic species populations, which is equal to the ratio of collisional-ionization to radiative-recombination rates, should be reduced by about the same amount as the ionization rate with respect to calculations assuming MB distribution (since there is little effect on the recombination rate). At higher densities (above 10^{21} cm⁻³ for low-Z plasmas), ionization is dominated by excitation-ionization cascades instead of direct ionization from the ground state.14 As the first excitation energy is typically (0.5-0.7) times the ionization potential, the reduction of ionization rates (and hence of the mean Z) should be significant, but less pronounced than for direct ionization. The strong reduction of excitation rates for high-energy transitions (high value of $\chi_{ij}/k_B T_e$) as opposed to the lesser effect on low-energy ones means that experimental diagnostics based on lines or line ratios will need to be reconsidered for laser plasma coronas.

Work is presently under way to study the effects of these rate modifications on atomic level populations using CRE (collisional radiative equilibrium) codes.

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