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Plasma density effects on the three-body recombination rate coefficients

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Abstract

The existing reaction rate coefficients for the three-body recombination of ions with plasma electrons have a strong $T^{-4.5}$ dependence on the electron temperature T, which seems to break down at low temperature, for $T < 1\ \mathrm{K} \simeq 10^{-4}$ eV. The obvious deficiency of the formula is the neglect of the plasma density effect on the recombined Rydberg states. A simple correctional procedure is adopted in terms of a density dependent cutoff of these high Rydberg states, which seems to improve the rates at low T. The total rate coefficients are now proportional to T^{-1}, for the density N not too low. The T dependence is closely related to the density, so that the -4.5 exponent is still valid at high T and low N region. Some numerical examples are given, and possible further improvements are suggested. The high and low T formulas interpolate smoothly through the principal quantum number cutoffs. © 1997 Published by Elsevier Science B.V.

1. Introduction

The temporal relaxation of a transient plasma toward a stationary state is dictated largely by the various reaction rates among the constituent electrons and ions. Thus, the ionization balance of a plasma is determined by the competing processes of ionization, recombination, and various excitation/de-excitation collisions, as well as radiative decays of excited states. In particular, the recombination of electrons and ions [1] takes place mainly by three different reaction modes, the radiative, dielectronic, and three-body recombinations (RR, DR, TBR, respectively). They are schematically described by

$$\begin{aligned} e + A^{Z+}(i) &\to A^{ZM+}(f) + x \quad (RR),\\ &\to A^{ZM+}(d) \to A^{ZM+}(f') + x' \quad (DR),\end{aligned}$$

$$e + e' + A^{Z+} \to A^{ZM+}(f'') + e'' \quad (TBR), \qquad (1)$$

where $ZM = Z - 1$, and f, f′ and f″ are the final ground or excited states which are only radiatively unstable, while states d denote doubly excited states which are Auger as well as radiatively unstable. Thus, in the TBR, the excess energy released by the recombining electron is carried away by the outgoing electron e″, $E_{e''} \simeq E_e + E_{e'} - E_{f'}$, so that the TBR does not involve any emission of photons, although f″ can cascade down radiatively once it is formed by the collisional process. On the other hand, in RR, $E_x = E_e + E_i - E_f$, and in DR the intermediate state d is in resonance with the initial configuration such that $E_e + E_i = E_d = E_{f'} + E_{x'}$. There are many cases in which the resonant modes can dominate [1], but in the following we neglect their contribution. Note that

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RR is the inverse of the direct photoionization, while the TBR is the inverse of the electron collisional ionization. These relations are often used in deriving the relevant cross sections, and we will also follow below the use of detailed balance.

The RR process is known to predominantly fill the low-lying Rydberg states, while the TBR is mainly responsible in rapidly bringing the high Rydberg states (HRS) into Saha equilibrium. Therefore, the TBR is an important process that determines the population of high-lying states. The current interest in the TBR stems from (i) the possibility [2,3] of creating in a laboratory the antihydrogen, where the cooled antiproton beam captures positrons in HRS via the TBR, which may then radiatively cascade down to lower hydrogenic states, and (ii) the prospect [4] for the formation of a ultra-cold plasma by laser irradiation of trapped cold atoms such that the ionized electrons are placed in the very low continuum states. The lifetime of such a transient plasma depends critically on how fast the continuum electrons recombine with the ions. The existing formulas for the TBR rate coefficients were derived for plasmas of temperatures typically in the range $T > 300$ K and relatively low electron density. The rate formula shows the strong $T^{-4.5}$ behavior, and this predicts rates which are clearly unphysical for $T < 1$ K. It is the purpose of this report to re-examine the formula for low temperature, and try to improve its behavior by including the possible density effect.

2. The TBR rate coefficients and the T dependence

In order to correct the TBR rate formula for the effect of plasma density, we first briefly review the simple arguments involved in the derivation of the existing rate formula. Although the detailed calculations carried out by several groups employed extensive numerical Monte Carlo, and rough classical arguments, the general behavior of the rates on T and N may be more simply understood. In the following, we use $T = T_e$ and $N = N_e$ interchangeably, as we will consider only the neutral plasma where $T = T_e = T_I$ and $N = N_e = N_Z$.

2.1. Collisional ionization rates

There are many useful empirical formulas for the collisional ionization rates, of varying degrees of reliability and regions of validity. We simply quote here one of the standard expressions [5,6],

$$\beta_{Z,n} \simeq 2.2 \times 10^{-8} N_Z N_e T_e^{1/2} e^{-x_n}(1 - e^{-x_n}) \times (I_{Z,n})^{-2} \Gamma_{Z,n} \quad (\mathrm{cm}^{-3}/\mathrm{s}), \tag{2}$$

where n is the principal quantum number of the captured electron, $x_n = I_{Z,n}/T_e$, Ry = 13.6 eV, $I_{Z,n} = Z^2/n^2$ Ry, and Γ is a Gaunt factor, which is of order 2. In the above formula, T and I are given in Ry s, and the densities N in units of cm^{-3}. As noted earlier, the above formula does not include the contributions from the resonant modes, which can be very large, especially when Z is small, $Z < 3$.

The following discussion of the TBR relies on the ionization formula (2). As such, the results we derive depend on the validity of the formula (2), especially for low T and high n. Since it is currently the most widely used, and probably the best available, rate formula, we simply adopt it in the following. Certainly, a more careful examination of this form (2) is warranted. (See also the discussion in Section 5.) We consider the two limiting cases of (2): First, (a) $x_n \gg 1$, i.e. for low T at a fixed n. Then

$$\beta_{Z,n}^{(a)} \simeq 2.2 \times 10^{-8} N_Z N_e T_e^{1/2} n^4 e^{-x_n} \Gamma_{Z,n}/Z^4 \quad (\mathrm{cm}^{-3}/\mathrm{s}), \tag{3}$$

where the n^4 factor comes from $I_{Z,n}^{-2}$ (and not from degeneracy). On the other hand, (b) for $x_n \ll 1$, corresponding to high T case for a fixed n, we have, instead of (3),

$$\beta_{Z,n}^{(b)} \simeq 2.2 \times 10^{-8} N_Z N_e n^2 e^{-x_n} \Gamma_{Z,n}/Z^2 T_e^{1/2} \quad (\mathrm{cm}^{-3}/\mathrm{s}), \tag{4}$$

which shows the distinct T and N behavior.

2.2.

The TBR rate coefficients are then obtained from (3) and (4) by detailed balance, as ($ZM = Z - 1$)

$$\alpha_{Z,n} = 3.3 \times 10^{-24} N_e (g_{ZM,n}/g_Z) e^{x_n}/T_e^{-3/2} \cdot \beta_{ZM,n} \times (\mathrm{cm}^{-3}/\mathrm{s}). \tag{5}$$

In (5), the degeneracy factors may be taken as $g_Z = 1$ and $g_{ZM,n} = n^2$. Then, for (a) with $x_n \gg 1$ at low T of interest here,

$$\alpha^{(a)}_{Z,n} \simeq 7.2\times 10^{-32} N_e^2 N_Z n^6 \Gamma_{Z,n}/q^4 T_e \text{ cm}^{-3}/\text{s}. \quad (6)$$

For (b) with $x_n \ll 1$ and at high T,

$$\alpha^{(h)}_{Z,n} \simeq 7.2\times 10^{-32} N_e^2 N_Z n^4 \Gamma_{Z,n}/T_e^2 Z^2 \ (\text{cm}^{-3}/\text{s}). \quad (7)$$

2.3.

The total TBR rates are obtained [7] by integrating the above rates for the individual n, as

$$\alpha^{\text{TBR}}_{Z,\text{tot}} \equiv \int_{n_0}^{n_{\max}} \alpha_{Z,n}\, \mathrm{d}n, \quad (8)$$

where n_0 is the lowest empty shell. The rate given by (8) is not sensitive to this value. The critical point in our discussion is in the choice of $n_{\max}$. The usual assumption is to choose for $n_{\max}$ the Thomson value, $n_{\max} \simeq n_T \simeq (T_e/Z^2\text{Ry})^{-1/2}$ associated with the thermal ionization of Rydberg electrons. Then, for the both cases (a) and (b) limits, we immediately obtain [8–10,7]

$$\alpha^{\text{TBR}-T(a)}_{\text{tot}} \simeq 1.1\times 10^{-31} N_e^2 N_Z Z^3 \Gamma_{Z,n}/T_e^{4.5} \ (\text{cm}^{-3}/\text{s}), \quad (9)$$

and $\alpha^{\text{TBR}-T(b)}_{\text{tot}} \simeq (0.77/1.1)\alpha^{\text{TBR}-T(a)}_{\text{tot}}$. All the existing TBR formulas exhibit this behavior, except for the slightly different numerical factors. The exponent -4.5 of T_e is the result of the strong n dependence, which comes from the degeneracy factor as well as the inverse square of the ionization energy.

3. The density effect and an improved rate formula

The plasma density effect is a complicated problem, and has been studied for many years in connection with the spectral broadening and ionization balance, and some aspects of the problem are still in a developing stage. For the present purpose of correcting the T, and possibly the N, dependence of the TBR rates, we adopt here a simple procedure for the determination of a density-dependent HRS cutoff $n_{\max}$ in (8). This procedure was employed earlier in Ref. [7]. Since we are mainly interested in the low T region with moderate densities, we simplify the discussion by setting $Z = 1$.

3.1.

We first consider [7] the several different ways by which the captured HRS are cut off. We define

$$n_{\max} = \min\{n_D, n_P, n_F, n_T\}, \quad (10)$$

where the various cutoffs are defined as follows: First, the Debye shielding radius is given [11] by $r_D = [T_e/4\pi N_e]^{1/2} = 5.15\times 10^{11}[T_e(\text{Ry})/N_e(\text{cm}^{-3})]^{1/2}$ (a_0), and thus

$$n_D = \sqrt{r_D/a_0} = 7.2\times 10^5\left[T_e(\text{Ry})/N_e(\text{cm}^{-3})\right]^{1/4}, \quad (11)$$

where a_0 is the Bohr radius. (As will be discussed below, the use of this n_D is predicated by the large plasma collision parameter Λ.) Next, the high n cutoff due to the particle packing n_P is defined in terms of the ion density which we are assuming to be $N_Z \simeq N_e$, as $(4\pi r_P^3/3)N_Z(\text{cm}^{-3}) \simeq 1$, which gives $r_P = 1.17\times 10^8[N_Z(\text{cm}^{-3})]^{-1/3}$ (a_0). This in turn gives

$$n_P = \sqrt{r_P/a_0} = 1.08\times 10^4\left[N_I(\text{cm}^{-3})\right]^{-1/6}. \quad (12)$$

This cutoff is independent of T_e and depends only weakly on the ion density. The principal quantum number cutoff due to the plasma microfield is estimated using the Holtzmark field and assuming that $r_F F_H = e/r_F$, where $F_H = 2.6|e|N_Z^{2/3}$ (a_0^{-3}) in a.u.. Therefore, we have $r_F = 2.6^{-1/2}[N_Z(a_0^{-3})]^{1/3}$ a_0. But, as noted previously [12], the Holtsmark field is accidentally nearly equal to the packing field, or, comparing the above two r's, r_P and r_F,

$$r_F \simeq r_P \quad \text{and} \quad n_F \simeq n_P. \quad (13)$$

Finally, the collisional cutoff by the thermal electrons is estimated by setting $2e^2/r_T \simeq k_B T_e(\text{Ry})$. This gives $r_T \simeq 2[k_B T_e(\text{Ry})]^{-1}(a_0)$, and thus

$$n_T \simeq \sqrt{r_T/a_0} \simeq 1.4\left[T_e(\text{Ry})\right]^{-1/2}. \quad (14)$$

This form (14) depends only on T_e and is independent of the density. It was used in the derivation of the $T_e^{-4.5}$ behavior.

3.2.

In evaluating the total TBR rate coefficients in the following we concentrate on the case (a) with $x_n \gg 1$ and low T. Since $\alpha_{\rm tot}$ of (8) is rather insensitive to n_0, we omit its discussion here. (Usually, $n_0 \leqslant 4$.) The Debye shielding cutoff $n_{\rm D}$ can be much smaller than $n_{\rm F}$ or $n_{\rm T}$. But, the use of $n_{\rm D}$ is valid in the region [11] where the plasma collision parameter $\Lambda \equiv N_{\rm e} r_{\rm D}^3 \gg 1$. This condition is often not satisfied by the kind of plasmas of interest here. Therefore, for the case (a) with (6), (8) and (12), and using $n_{\max} = n_{\rm F}$,

$$\alpha_{\rm tot}^{\rm TBR-\mathit{F}(\mathit{a})} \simeq 1.8 \times 10^{-4} [T({\rm Ry})]^{-1} N_{\rm e}^{5/6} N_z \Gamma_{Z,n} Z^{-4} \quad ({\rm cm}^{-3}/{\rm s}). \tag{15}$$

This is the main result of this report, and should be compared with Eq. (9) of Section 2. It is important to keep in mind that (15) is valid in the limit $n_{\rm F} \simeq n_{\rm P} < n_{\rm T}$, while (9) is valid for $n_{\rm F} > n_{\rm T}$.

We further define the total transition probability P by

$$P_{\rm tot}^{\rm TBR} \equiv N_{\rm e}^{-1} \alpha_{\rm tot}^{\rm TBR} \quad ({\rm s}^{-1}). \tag{16}$$

Insofar as the case (b) is concerned, we may have $\alpha_{\rm tot}^{\rm TBR-\mathit{F}(\mathit{b})} \simeq 2.1 \times 10^{-12}\ T_{\rm e}^{-2}\ N_{\rm e}^{7/6} N_Z \Gamma_{Z,n} Z^{-2}$ $({\rm cm}^{-3}/{\rm s})$. However, we recall that this formula was derived using the conditions $x_n \ll 1$ and $n_{\rm F} < n_{\rm T}$. The condition $x_n \ll 1$ is equivalent to $n > n_x$, where $n_x = T_{\rm e}^{-1/2} \simeq n_{\rm T}$. Therefore, the two conditions are mutually orthogonal and the allowed range of n is zero. Therefore, the TBR-$F(b)$ case does not exist.

4. Numerical examples

To illustrate the use of the new rate formula (15) that roughly incorporates the plasma density effect and to compare it with the rates given by (9), we consider a typical case

$$T_{\rm e} \simeq 10^{-7} {\rm Ry} \simeq 0.16\ {\rm K},$$

$$N_{\rm e} \simeq N_{\rm I} \simeq 10^{11}\ {\rm cm}^{-3},$$

with $Z = 1$ for the charge of the ions. We also assume for simplicity $N_{\rm e} \simeq N_Z$.

First, we evaluate the cutoff parameters associated with the different physical assumptions. For the above plasma parameters, we have

$$n_{\rm D} \simeq 23, \quad n_{\rm F} \simeq n_{\rm P} \simeq 160, \quad n_{\rm T} \simeq 4400.$$

Obviously, the thermal cutoff n is very large and physically unrealistic, while, due to the plasma collision parameter $\Lambda \simeq 2 \times 10^{-6} \ll 1$, the Debye shielding cutoff is not applicable. Therefore, $n_{\max} \simeq n_{\rm F}$, and the total TBR transition probability is given by (15) and (16)

$$P_{\rm tot}^{\rm TBR-\mathit{F}(\mathit{a})} \simeq 5.2 \times 10^{12}\ {\rm s}^{-1},$$

which is to be compared with the prediction by the previous formula (9) and (16); i.e.

$$\alpha_{\rm tot}^{\rm TBR-\mathit{T}(\mathit{a})} \simeq 6.8 \times 10^{22}\ {\rm s}^{-1}.$$

This value is quite unrealistic and thus (9) breaks down in this case. On the other hand, the value with the TBR-$F(a)$ is within the physically acceptable range. Obviously, there is a factor of 10^{10} difference in the predicted rates. For case (b), we have $P_{\rm tot}^{\rm TBR-\mathit{T}(\mathit{b})} \simeq 4.9 \times 10^{22}\ {\rm s}^{-1}$ and $P_{\rm tot}^{\rm TBR-\mathit{F}(\mathit{b})} \simeq 2.9 \times 10^{15}\ {\rm s}^{-1}$; again a factor of 10^7 reduction is involved here, but both these values seem to be unrealistically high. More seriously, however, as discussed earlier, the TBR-$F(b)$ case is not valid. For comparison, we also quote the total RR rate coefficients for the above parameters,

$$\alpha_{\rm tot}^{\rm TBR} \simeq 10\ {\rm s}^{-1}.$$

For a slightly different set of parameters, for example, $T_{\rm e} \simeq 1$ K and $N_{\rm e} \simeq N_Z \simeq 10^8\ {\rm cm}^{-3}$, we obtain a more reasonable rate, $\alpha_{\rm tot}^{\rm TBR-\mathit{F}} \simeq 10^8\ {\rm s}^{-1}$.

We present in Fig. 1 the $N_{\rm e}$ and $T_{\rm e}$ dependence of the cutoff $n_{\max}$ for ready determination of the validity region for (15) and (9). The regions below the solid curve are for formula (15), while the region above the curve is for (9). The dependence of the TBR rate coefficients on T and N is illustrated in Fig. 2, where the predictions of the TBR probabilities by formulas (9) and (15) are illustrated. To show further the interplay between the T and N dependence of the transition probability P and the use of the two figures, we consider for example $T_{\rm e} = 10^{-5}$Ry and $N_{\rm e} = 10^7\ {\rm cm}^{-3}$. From Fig. 1, we have $n_{\rm T} < n_{\rm F}$, so that immediately the formula (9) is valid in this case, with $P = 7 \times 10^5\ {\rm s}^{-1}$ from Fig. 2. On the other hand, for $N_{\rm e} = 10^9\ {\rm cm}^{-3}$ and at the same T, we have $n_{\rm F} < n_{\rm T}$ and $P = 1.1\% \times 10^9\ {\rm s}^{-1}$, again

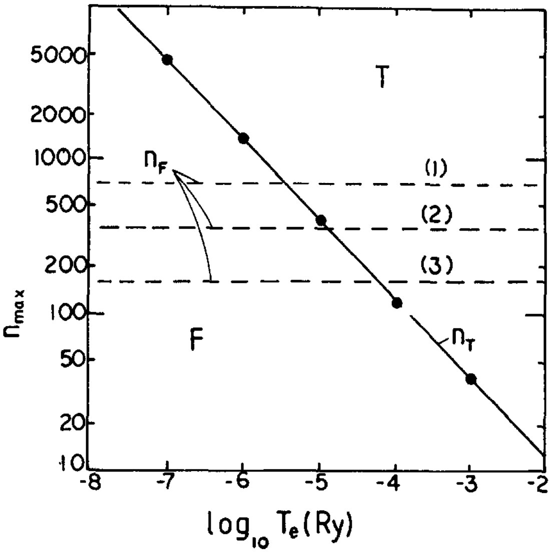

Fig. 1. The $T = T_e$ and $N = N_e$ dependence of the cutoff parameter $n_{max} = n_T$ or n_F is shown; formula (9) is valid in the region $n_T < n_F$ and (15) is to be used for $n_F < n_T$. The region below the solid curve for n_T is for (15) and the region above is for (9). Curves (1), (2) and (3) are for the electron densities; (1) for $N_e = 10^7$ cm^{-3}, (2) for $N_e = 10^9$ cm^{-3}, and (3) for $N_e = 10^{11}$ cm^{-3}.

from Fig. 2. Generally, for $T_e < 10^{-6}$Ry, (15) is valid for all $n_e > 10^5$ cm^{-3}. But for $T_e > 10^{-4}$Ry, (9) is valid for all $N_e < 10^{11}$ cm^{-3}. Thus, generally the formula (9) is valid for high T and low N, while (15) is applicable for low T and high N. The two regions are divided by the solid line for n_T in Fig. 1.

We also estimated the Debye shielding parameters for the T and N values of interest here. With $N_e = 10^9$ cm^{-3} and $T_e = 10^{-7}$Ry, we have $n_d \simeq 45$ and $\Lambda \simeq 10^{-12}$. For the $N_e = 10^{11}$ cm^{-3} at the same temperature, we obtain $n_d \simeq 24$ but $\Lambda \simeq 2 \times 10^{-10}$. For the parameter range of interest here, Λ is in most cases very small, and thus the use of n_D is not appropriate.

5. Ionization threshold problem

It is important to point out that the TBR problem is closely related to the Wannier threshold [13] problem, where the TBR is an inverse of the collisional ionization. Since both (9) and (15) depend on the validity of (2), more careful examination of the ionization rate β is needed, especially in the untested region of very low T and high n. The energy dependence of the cross section near the threshold determines the T dependence; the Wannier prediction of $\sigma^{\text{Ionis}} \simeq E_c^{\gamma}$, with $\gamma = \gamma_W \simeq 1.127$, may be compared with the Coulomb asymptotic value $\gamma_{cou} \simeq 1.00$, and the dipole value [14], $\gamma_{dipole} \simeq 1.50$. However, the more important question is the available phase space to which two continuum electrons are placed, since all three types of asymptotic behavior are allowed in the solution. (The common misconception that the dynamics specified by the Schrödinger equations should determine the value of γ is not correct, since the asymptotic boundary conditions must be imposed separately from the equation of motion. Whether one kind of boundary condition represents the experimental situation is a separate

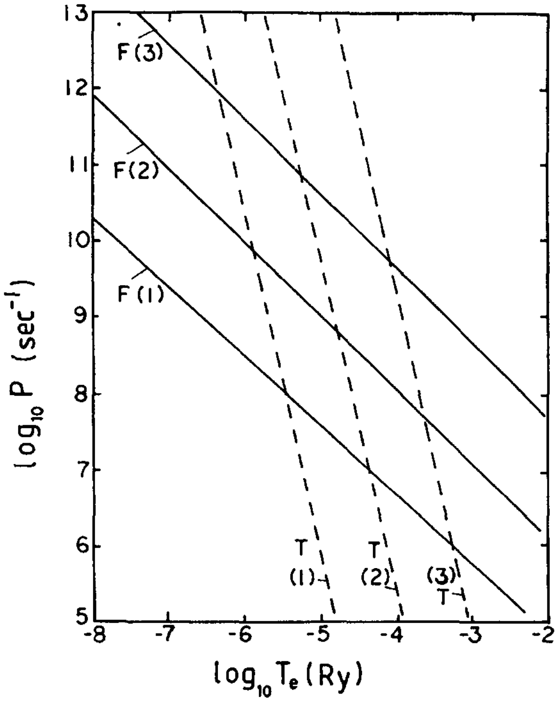

Fig. 2. The density and temperature dependence of the newly derived TBR rate formulas (9) and (15) is exhibited, for different $N = N_e$ and $T = T_e$ combinations. The solid lines are for TBR-F and the formula (15), while the dashed lines are for TBR-T of (9), at three different densities; (1) for $N_e = 10^7$ cm^{-3}, (2) for $N_e = 10^9$ cm^{-3}, and (3) for $N_e = 10^{11}$ cm^{-3}. The sharp T dependence of the TBR-T curves is evident, due to the $T^{-4.5}$ behavior of the probability P.

matter.) Experimental investigation of the T and N dependence of the cold plasma, as described by the old formula (9) or by the modified form (15), should help understand the threshold behavior of the ionizing three-body system.

6. Summary

An improved formula for the total TBR rates is presented which seems to be more reasonable for low T and moderate to high density plasmas. It is obtained by approximately including the plasma density effect through the HRS cutoff. The T dependence is drastically modified, from the previous $T^{-4.5}$ to a more moderate T^{-1}, with the corresponding change in the density depndence as well. Therefore, we have the new formula (15) for the case $n_F < n_T$, while the form (9) is still valid in the parameter region $n_T < n_F$.

The numerical examples suggest that with proper adjustments of the T and N parameters, it may be feasible to produce a very low temperature plasma. (Such plasmas are usually very strongly coupled [15], with the coupling parameter $\Gamma_{\text{plasma}} \simeq e^2/(r_P \cdot k_B T_e) \gg 1$.) The TBR plays an important negative role, especially in filling the HRS and bringing them rapidly to Saha equilibrium, thus destroying the plasma. But, with smaller TBR rates, and much slower RR rates, it may be possible to produce a transient cold plasma and maintain it long enough to be able to perform experiments with it.

On the other hand, the anti-hydrogen production depends on the TBR rates, in the positive sense that for faster TBR rates more antihydrogens are produced, as the positrons are captured first by the anti-protons to HRS and then cascade down to lower states either by collisions or by radiative relaxation. Therefore, the new rates places different limitations on the estimate of producing such exotic systems.

As stressed earlier, the derivation of the new rate formula and re-interpretation of the old one are crude and approximate. The plasma density effect is a complex problem that requires further careful study, both experimentally and theoretically, especially in the low temperature regime. The forms presented here, (9) and (15), must therefore be regarded as preliminary, but the main essential physics seems to be incorporated correctly. The principal shortcoming of the simple treatment of the density effect given here is the possible coherent effect of the continuum electron at very low temperature with very long de Broglie wave length and the presence of many ions within this wavelength. This may further adjust the density dependence of the TBR probability. More careful theoretical analyses and experimental study are needed to further improve the rate formulas if high accuracy is required. For strongly coupled plasmas, much work has been carried out using a variety of techniques [16], notably by Bierman et al. [17] using the Fokker–Planck equations, and by the Rostock group [18,19] using many-body Green functions. However, extensions of their work to the very low T and high n regime may be difficult.

The main part of the needed adjustment in the TBR rates has been achieved by the result of this report, to the extent that one can now reliably estimate the contribution of the TBR at low temperature and high Rydberg states for much of the current applications.

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