SHOCK RADIATION RECOMBINATION AS A DIFFUSION PROCESS

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The quasistationary process of shock radiation recombination is described by a stationary diffusion equation which is solved under the assumption of a constant current and taking account of the exact dependence of the diffusion and drift coefficients on the number of the atomic energy level. A comparison is made with the results of other authors obtained by other methods.

The recombination rate is defined by the resultant rate of electron capture by ions and can be found only by taking account of the kinetics of filling the atom (ion) levels.

Since single-electron processes predominate, the atom (ion) formed at any time as a result of electron capture can be considered as a single-electron system, and the plasma, correspondingly, can be characterized by statistical single-level amplitudes, the relative concentrations $\alpha_{kn} = N_{kn}/N$, where N_{kn} is the concentration of ions with the charge $k = 0, 1, 2, \ldots, z$ in the state $n = 1, 2, \ldots$, $N = \sum_{kn} N_{kn}$ is the total concentration of all the ions. The charge distribution is determined by the charge amplitudes $\alpha_k = \sum_n \alpha_{kn}$. The degree of ionization α (the number of electrons per ion) is the first moment of this distribution

$$\alpha = \sum_k k\alpha_k = \sum_{kn} k\alpha_{kn}. \tag{1}$$

Conservation of the total charge is equivalent to normalizing the amplitude:

$$\sum_{kn} \alpha_{kn} = \sum_k \alpha_k = 1. \tag{2}$$

For the single ionization considered below, $k = 0$ and 1, which cannot be considered excited ion states under the single-electron processes conditions (this is dictated by the transition matrices $kn \rightleftharpoons k'n'$) so that taking account of (1) and (2), we obtain

$$\alpha_1 = \sum_n \alpha_{1n} = \alpha = 1 - \alpha_0 = 1 - \sum_n \alpha_{0n}. \tag{3}$$

It is convenient to represent the kinetic equations for the distribution of α_{0n} over the atom levels as

$$\dot{\alpha}_{0n} = \sum_{n'} (K_{n'}^{n'} \alpha_{0n'} - K_n^{n'} \alpha_{0n}) + q_n, \quad q_n = K_n^{\infty}(A\bar{\alpha}_{0n} - \alpha_{0n}), \quad A = \frac{\alpha^2}{\bar{\alpha}^2}. \tag{4}$$

The summation is here performed over all states n' interacting with the central state n. For convenience, the transitions in the continuum and back ($n \rightleftharpoons \infty$) are isolated, where the capture rate K_{∞}^{n} (a ternary process) is expressed in terms of the ionization rate (a pair process) by using the principle of detailed equilibrium. Here $\bar{\alpha}$ and $\bar{\alpha}_{0n}$ are equilibrium quantities defined by the Saha and Boltzmann formulas.

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The transition rates over the discrete levels $K_n^{n'}$ $(n \to n')$ are represented by the sums of the electron $\overset{e}{K}{}_n^{n'}$ and radiation $\overset{r}{K}{}_n^{n'}$ transition rates (recombination in an optically thin plasma is considered here). For hydrogen-like atoms we have (see [1], for example)

$$\overset{e}{K}{}_n^{n'} = 2\cdot 10^{-6}\alpha N T_e^{-1/2}\frac{e^{x_{nn'}} - x_{nn'}E_e(x_{nn'})}{n^5 n'^3 (n^{-2}-n'^{-2})^4}, \quad n' > n, \quad x_{nn'} = (n^{-2}-n'^{-2})\,I/T_e; \tag{5}$$

$$\overset{e}{K}{}_n^{\infty} = 2{,}4\cdot 10^{-8}\alpha N T_e^{-1/2} I n^2 [e^{-x_n} - x_n E_e(x_n)], \quad x_n = I/T_e n^2; \tag{6}$$

$$\overset{r}{K}{}_n^{n'} = 1{,}6\cdot 10^{10} n^{-3} n'^{-1}(n^2 - n'^2)^{-1}, \quad n' < n; \tag{7}$$

$$\overset{e}{K}{}_{n'}^{n} = \left(\frac{n}{n'}\right)^2 e^{x_{nn'}}\overset{e}{K}{}_n^{n'}, \quad n' > n. \tag{8}$$

The last formula has been obtained by using the principle of detailed equilibrium. The energy and temperature are in eV in all the formulas, and $E_e(x) = \int_x^\infty e^{-x}dx/x$ is the exponential integral.

Analysis shows that the electron and photon processes can be represented sufficiently accurately by transitions just between adjacent states [2], i.e., by the transitions $n \rightleftharpoons n \pm 1$. In this case the diffusion method is represented by the following equation [2]:

$$\tau_n \ddot{\alpha}_{0n} + \dot{\alpha}_{0n} = \frac{\partial^2}{\partial n^2}(D_n\alpha_{0n}) - \frac{\partial}{\partial n}(U_n\alpha_{0n}) + q_n. \tag{9}$$

This hyperbolic diffusion equation describes diffusion at a finite rate $K_n = \sum_{n'} K_n^{n'} = \tau_n^{-1}$ $(\sec^{-1})$ and goes over into the Fokker – Planck parabolic diffusion equation as $K_n \to \infty$ $(\tau_n \to 0)$, where τ_n is the expectation time of the transition from the state n. The diffusion D_n and drift U_n (the mean velocity of motion along the n axis) coefficients are expressed in terms of the transition velocities $K_n^+ = K_n^{n+1}$ and $K_n^- = K_n^{n-1}$ ahead of and behind the n axis by the following formulas

$$D_n = \frac{1}{2}(K_n^+ + K_n^-), \quad U_n = K_n^+ - K_n^-. \tag{10}$$

Differentiating (3) we obtain

$$\dot{\alpha} = -\sum_n \dot{\alpha}_{0n}. \tag{11}$$

It hence follows that the ionization – recombination process is essentially nonstationary ($\dot{\alpha} = 0$ follows from $\dot{\alpha}_{0n} = 0$) and can be described correctly only by the nonstationary system (4) or by representing it by the diffusion equation (9). Under quasistationarity conditions, when the rate of filling the ground level (n = 1) is low, the recombination process can be described (approximately it is understood) by the stationary diffusion equation

$$-\frac{\partial j_n}{\partial n} = (D_n\alpha_{0n})'' - (U_n\alpha_{0n})' = -q_n. \tag{12}$$

In this case the population of the ground level can be considered an equilibrium (Boltzmann) population:

$$\alpha_{0n}(n=1) = \bar{\alpha}_{0n}(n=1). \tag{13}$$

This expression is the boundary condition for (12).

The representation of ternary recombination by a stationary diffusion equation of Fokker – Planck type was first realized by Pitaevskii [3, 4], however, he used the limit expression for the diffusion coefficient $D_n \sim n^4$, which is applicable only for high levels $(n \gg \bar{n} = (I/T_e)^{1/2})$, or for comparatively low temperatures and high densities. The diffusion method described above affords the possibility of using exact dependence of the drift and diffusion coefficients on the number of the atom energy level n and of therefore obtaining the

recombination coefficient for any temperatures and densities. It should be emphasized that the radiation transitions essential for recombination (in the problem formulation under consideration) were used by Pitaevskii in the form of the boundary condition $\alpha_{0n} = 0$ in place of (13). This is possible only in the strong recombination mode ($A \gg 1$), however, the quasistationarity condition can be spoiled for large A.

Since the oppositely directed capture K_{∞}^{n} and ionization K_{n}^{∞} rates grow abruptly with n, a quasistationary ionization equilibrium is set up at the upper levels. Setting $q_n = K_n^{\infty}(A\bar{\alpha}_{0n} - \alpha_{0n}) = 0$, we obtain the second boundary condition as $n \to \infty$:

$$\alpha_{0n} = A\bar{\alpha}_{0n}; \quad A = \frac{\alpha^2}{\bar{\alpha}^2} \quad (n \to \infty) \tag{14}$$

(the quasistationary distribution is a Boltzmann distribution $\bar{\alpha}_{0n}$ at the upper levels since the transition velocities at sufficiently high levels are determined only by electron processes).

The expression (14) is applicable in practice for $n > \bar{n} = (I/T_e)^{1/2}$.

It is possible to simplify (12) if it is taken into account that the source q_n is located at the upper levels ($n \gtrsim \bar{n}$) and the fundamental electron time is expended in motion at the low levels. This affords a foundation for not considering the source distribution $q_n = q(n)$ but to concentrate it at the upper levels ($n \gg \bar{n}$), i.e., actually to combine it with the upper boundaries. If the source makes the transition to the boundary, then we should set $q_n = 0$ in the equation. In this case the current over the levels turns out to be constant, i.e., $j_n = -(D_n\alpha_{0n})' + U_n\alpha_{0n} = j = \text{const}$ and we obtain a first-order equation in place of (12) which it is convenient to represent as

$$\beta'_{0n} - \beta_{0n}\tilde{\beta}'_{0n}/\tilde{\beta}_{0n} = -j \tag{15}$$

in terms of the variable

$$\beta_{0n} = \alpha_{0n}D_n, \tag{16}$$

and the solution $\tilde{\beta}_{0n}$ of (15) for zero current ($j = 0$) with the boundary condition $\tilde{\beta}_{0n} = \bar{\beta}_{0n}$ as $n \to \infty$.

The solution of (15) with the above-mentioned boundary conditions is

$$\beta_{0n} = \tilde{\beta}_{0n}\left[A + j\int_{n}^{\infty} dn/\tilde{\beta}_{0n}\right], \tag{17}$$

where

$$j = -(A-1)\Big/\int_{n_0}^{\infty} dn/\tilde{\beta}_{0n} \tag{18}$$

is the total (effective) current. Under quasistationary conditions, the lower limit can be extended to $n_0 = 2$, and even to $n_0 = 1$ for constant current.

Pitaevskii obtained a solution of an equation of the type (15) with $j = \text{const}$ and for $A \gg 1$ (under strong recombination conditions). As is easy to see, his solution corresponds to neglecting the ionization current (the second member in (18)) or the boundary conditions $\alpha_{0n} = 0$ for $n = n_0$ in place of the more common (13). It should be kept in mind that separation of the current into ionization and recombination currents is impossible in the general case for finite A.

The solution (17) is more general. The dependence on the density is contained therein in terms of the drift and diffusion coefficients (taking account of the radiation transitions in exact form). It is applicable down to the lowest levels because of taking account of the dependences of the diffusion equation parameters on n exactly, which is quite important, as will later be clear, since such levels for which it is impossible to use the limit expression of the diffusion coefficient (as $n \to \infty$) yield a contribution to the recombination current.

The results of a computation are presented in Fig. 1 in the form of the ratio $\gamma = \beta_P/\beta_T$ between the recombination coefficient β_P obtained by Pitaevskii as $N_e \to \infty$ and with the limit dependence $D_n \sim n^4$ and the recombination coefficient β_T obtained by means of (18) with the exact dependence of D_n on n and taking account of the radiation transitions. Such a mode of representing the results is convenient in that it does not contain a numerical factor in the diffusion coefficient (upon agreement of the coordinate dependences of the expression presented here and the classical expression for the Pitaevskii diffusion coefficient as $n \to \infty$,

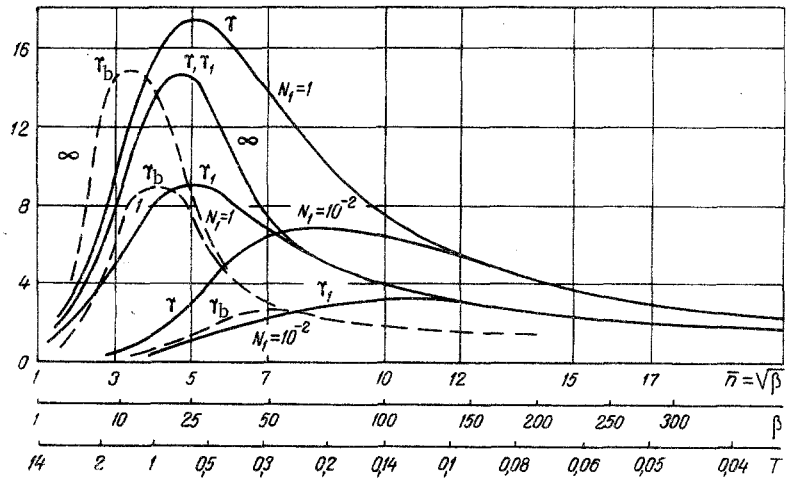

Fig. 1. Temperature dependence of the correction factor to the Pitaevskii recombination coefficient. The curve γ corresponds to the quasistationary distribution $\tilde{\alpha}_n$ and the curve γ_1 to the Boltzmann distribution. The dashed curves are the appropriate Bates results.

the numerical factor in this latter is divided by four). The graphs represent the temperature dependence $\gamma(T_e)$ for diverse fixed electron concentrations $N_e = \alpha N$ (N is presented in the units 10^{16} cm^{-3} so that $N_1 = N \cdot 10^{-16}$). The Pitaevskii result corresponds to the limit $N \to \infty$ and is realized in practice for $N_1 \gtrsim 10^3$. The ratio between the recombination coefficient obtained by means of (18), with the quasistationary distribution $\tilde{\alpha}_{0n}$ replaced by a Boltzmann distribution $\bar{\alpha}_{0n}$ applicable for a dense plasma, is presented for the same concentration values for comparison. The corresponding curves are denoted by γ_1. The magnitude of the current depends on the population α_{0n} and the diffusion coefficient D_n.

The recombination coefficient obtained by the method considered here turns out to be less than the Pitaevskii value. It is essential that the recombination coefficient remain approximately one-half the Pitaevskii value even at comparatively low temperatures ($T_e \sim 0.1$ eV) when the diffusion method is applicable in the Fokker–Planck form. This difference is due to the application of the limit expression for the diffusion coefficient ($D_n \sim n^4$), which is suitable only for high levels (for $n \gg \bar{n}^{2/3}$) while the domain $n \lesssim \bar{n}$ in which the exponent is on the order of one yields the main contribution to the current integral. This circumstance is illustrated in Fig. 2, where it is shown how the current integral (sum) s_1 is collected at the upper limit n. The curves s_2 yields the Pitaevskii integral for the same values of $\beta = x_1$. Let us note that the maximum of the integrand in the Pitaevskii form holds for $n = \bar{n}/\sqrt{3} < \bar{n}$, which indicates the inapplicability of the limit expression for the diffusion coefficient. As a rule, up to 90-95% is collected up to 90-95% for $n \leq \bar{n}$, and s_2 up to 85-90%. As an estimate shows, the limit expression for the diffusion coefficient can be used only at the temperatures $T_e \lesssim$ 100-150°C (the estimate of the level range is given above).

The dashed curves in Fig. 1 illustrate the Bates results [5] obtained by numerical solution of the system of kinetic equations (4) with a finite number of levels (quasistationary version). These results have been obtained with a different expression for the transition velocity, hence for comparison they are normalized to the value obtained here for $T_e \sim 1$ eV, where the correction coefficient turns out to be on the order of 1. The maximum values of the correction coefficients agree, in practice, for all concentrations, and the positions of the maximums diverge somewhat. Quasistationarity is spoiled for $T_e > 0.7$ eV so that the recombination coefficient is not representative in this domain.

It is interesting to note the following. The exact expression for the current in the stationary model is obtained from (12) as

$$j_n = -\int_n^\infty q_n dn = -\int_n^\infty K_n^\infty (A\bar{\alpha}_{0n} - \alpha_{0n})\, dn. \tag{19}$$

For the total capture rate we obtain

$$q = \int_{n_0}^\infty K_n^\infty (A\bar{\alpha}_{0n} - \alpha_{0n})\, dn = -j_n(n_0). \tag{20}$$

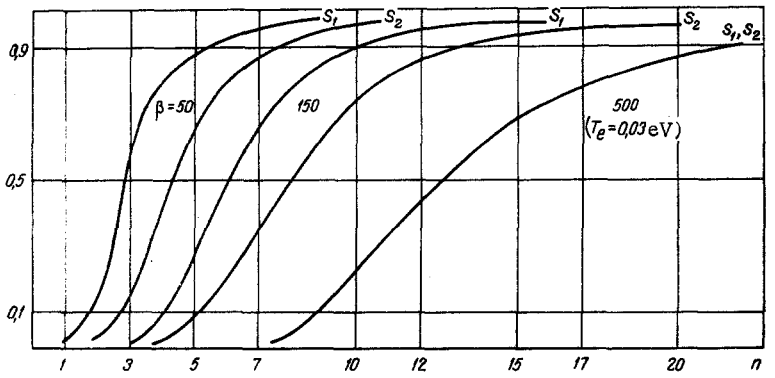

Fig. 2. Dependence of the current normalized to one on the upper limit of the integral (sum). The curve s_1 is the integral in the form (18) while the curve s_2 is the Pitaevskii integral. $\beta = I/T_e$.

Since the contribution to the current is slight for $n \gg \bar{n}$, let us limit ourselves approximately to integration to $n = \bar{n}$, which Hinnov and Hirschberg [6] used to evaluate the recombination coefficient by means of the formula

$$j_{rec} = \int_{n_0}^{\bar{n}} K_n^{\infty} A \bar{\alpha}_{0n} dn \qquad (21)$$

with the integral also replaced by a sum at the lower levels. Their results for a dense plasma agree with the Pitaevskii results to the accuracy of a numerical factor of ~0.5. Although it is impossible to consider such results sufficiently exact (the model selection of the upper limit), their method yields a numerical result which practically agrees with that obtained here (in the dense plasma limit). Let us emphasize that the agreement between the temperature dependences of the recombination coefficient in the Hinnov–Hirschberg and Pitaevskii methods (the formulas for the computation are completely different) is random and related to the specific dependence of the diffusion coefficient on n ($D_n \sim n^4$) and the ionization rate $K_n^{\infty} \sim n^2$ (the exponents in these expressions just influence the numerical factor).

The fact that the expression (18) for the current differs in form from the exact expression (19) suggests the need to solve the exact stationary (second-order) diffusion equation in place of the approximate (first-order) equation. However, because of the modeling of the stationary problem it is not clear in advance whether the results are improved.

Let us note that an attempt to correct the Pitaevskii results by a summation over discrete levels (for extension to high temperatures) was made by Biberman et al. [7], where only the transition $n = 1 \rightleftharpoons 2$ was realized. It is impossible to extend the current integral in the Pitaevskii form (even represented as a sum) to the low levels for the reasons mentioned above, hence, the mentioned correction is qualitative (interpolational) in character.

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