ELECTRON RECOMBINATION IN A WEAKLY IONIZED GAS

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The recombination coefficient between electrons and ions in triple collisions in a neutral gas is calculated. The calculation is performed on the basis of the Boltzmann equation. The result is close to the Thomson value.

IN a highly rarefied plasma the main mechanism of recombination is radiative. In a rather dense plasma, recombination processes with participation of a third particle become dominant. For a high degree of ionization, electrons constitute third particles of this type.[1-4]

In a weakly ionized gas a triple collision of the recombining particles with a neutral atom is the most probable. An elementary calculation of the recombination coefficient α for this case was first made by Thomson.[5] The same problem was solved by Pitaevskiĭ[6] by means of the Fokker-Planck equation. Pitaevskiĭ's result differs from that given by Thomson by a numerical factor.

In the work being presented the recombination coefficient will be calculated on the basis of Boltzmann's classical kinetic equation for electrons. For the classical description to be possible it is necessary that the electron energy E be small in comparison with the first Bohr level $m_1e^4Z^2/\hbar^2|E| \gg 1$ (m_1 is the electron mass, eZ is the ionic charge, $\hbar$ is Planck's constant).[7] We will limit the discussion to the case of a plasma in thermal equilibrium, $\overline{E} \sim T$ ($\overline{E}$ is the thermal energy of the electrons, T is the temperature of the neutral gas and ions).

To calculate α it is necessary to find the electron flux to an ion moving with a velocity v_i in the plasma, and then to average this flux over the thermal distribution of the ions:

$$F_i(v_i) = \left(\frac{m_2}{2\pi T}\right)^{3/2} \exp\left(-\frac{m_2 v_i^2}{2T}\right), \qquad (1)$$

where m_2 is the mass of the atom and the mass of the ion.

The motion of an electron in the field of a positively charged ion can be both infinite ($E > 0$) and finite ($E < 0$). In a rarefied plasma, if we neglect collisions, the kinetic equation for electrons in a Coulomb field is easily solved; the corresponding distribution function depends on the integrals of motion—on the energy and momentum. In this approximation there is no flux of particles to the center.[8] When collisions are included, if they are rather infrequent, the concept of finite particles is preserved. However, as the result of collisions, they can now fall on the center. The flux arising in this way is proportional to the frequency of collisions. To calculate this flux for $\delta e^4Z^2/T^2l^2 \ll 1$ ($\delta = 2m_1/m_2$, l is the electron mean free path in the neutral gas) we will simplify the kinetic equation by means of the method of Budker and Belyaev, which consists of averaging over the fast motion of finite particles.[9,10]

It is convenient to carry out the entire discussion in a coordinate system tied to an ion moving with respect to the gas with a velocity v_i. In the kinetic equation for the electron distribution function $f(\mathbf{r}, \mathbf{v}, t)$,

$$\frac{\partial f}{\partial t} + (\mathbf{v}\nabla)f + \frac{\mathbf{Q}}{m_1}\frac{\partial f}{\partial \mathbf{v}} = \mathrm{St}, \qquad (2)$$

there remains only the integral of elastic collisions with the neutral gas:

$$\mathrm{St} = \int [f(\mathbf{v}_1')F(\mathbf{v}_2') - f(\mathbf{v}_1)F(\mathbf{v}_2)]\,\sigma v_0\, d\mathbf{v}_2\, d\mathrm{o}. \qquad (3)$$

Here $\mathbf{v}_0 = \mathbf{v}_1 - \mathbf{v}_2$ is the relative velocity of the colliding particles, $d\mathrm{o} = \sin\chi d\chi d\varphi$ is the element of solid angle into which the scattering occurs, $\sigma(v_0, \chi)$ is the differential cross section for scattering, and $\mathbf{Q} = e^2Z\mathbf{r}/r^3$.

We will assume the distribution function of the molecules to be Maxwellian:

$$F(\mathbf{v}_2) = n_2\left(\frac{m_2}{2\pi T}\right)^{3/2} \exp\left(-\frac{m_2(\mathbf{v}_e + \mathbf{v}_i)^2}{2T}\right), \qquad (4)$$

where n_2 is the number of molecules (atoms) per cubic centimeter.

The particle velocities before the collision ($\mathbf{v}_1$, $\mathbf{v}_2$) and after the collision ($\mathbf{v}_1'$, $\mathbf{v}_2'$) are related by

expressions based on conservation of momentum and energy:

$$\mathbf{v}_1' = \mathbf{v}_1 + \frac{1}{m_1}\Delta, \quad \mathbf{v}_2' = \mathbf{v}_2 - \frac{1}{m_2}\Delta, \tag{5}$$

$$v_0 = v_0' = (v_1^2 - 2(\mathbf{v}_1\mathbf{v}_2) + v_2^2)^{1/2},$$

$\mathbf{v}_0' = \mathbf{v}_1' - \mathbf{v}_2'$ is the relative velocity of the particles after the collision. The momentum transfer Δ is expressed in terms of the reduced mass $M = m_1m_2/(m_1 + m_2)$, the unit vector $\nu = (\mathbf{v}_0 - \mathbf{v}_0')/v_0$, and the scattering angle χ by the simple formula

$$\Delta = -2Mv_0\nu\sin\frac{\chi}{2}. \tag{6}$$

The electron energy E changes in a collision with a molecule by an amount

$$\varepsilon = E' - E = -2Mv_0v_2\sin\frac{\chi}{2}\cos(\widehat{v_2\nu}) - 2\frac{M^2}{m_2}v_0^2\sin^2\frac{\chi}{2}$$

$$= -2Mv_0v_1\sin\frac{\chi}{2}\cos(\widehat{v_1\nu}) + 2\frac{M}{m_1}v_0^2\sin^2\frac{\chi}{2}. \tag{7}$$

In the collision of an electron with a molecule, the electron velocity changes markedly (by the order of magnitude of unity), and the momentum changes correspondingly. The energy changes insignificantly (by the order of magnitude $\sqrt{m_1/m_2}$). For this reason a small number of collisions is sufficient to attain the equilibrium value of the momentum μ. The rapidly established equilibrium value of μ is completely determined by the electron energy, $\mu = e^2Z(m_1/2|E|)^{1/2}$. Consequently, the only slow variable on which the distribution function depends is the energy of the electron relative motion E.

By averaging Eq. (2) over the rotational motion, we obtain the equation for the distribution function of finite electrons f(E, t):

$$\frac{\partial f}{\partial t} = \int [f(E')\overline{F(E_2')} - f(E)\overline{F(E_2)}]\sigma v_0 d\mathbf{v}_2 do. \tag{8}$$

Since f does not depend on the direction of the velocity $\mathbf{v}_i$, we can also average over this direction in Eq. (8). Here

$$v_2 = (2E_2/m_2)^{1/2},$$

$$\overline{F(E_2)} = \frac{1}{2}\int_{-1}^{1} F(\mathbf{v}_2)\,d\cos(\widehat{v_2v_i})$$

$$= n_2\left(\frac{m_2}{2\pi T}\right)^{3/2}\frac{T}{m_2v_iv_2}\operatorname{sh}\left(\frac{m_2v_iv_2}{T}\right)$$

$$\times\exp\left(-\frac{m_2(v_2^2 + v_i^2)}{2T}\right). \tag{9}$$

In finite orbits

$$v_1^k = \left(\frac{2|E|}{m_1}\right)^{k/2}, \quad r^n = \left(\frac{e^2Z}{2|E|}\right)^n, \tag{10}$$

where k and n are arbitrary.

If we utilize the fact that $\sqrt{m_1/m_2}$ is small, the accurate formulas (5) and (7) can be converted to the following approximate formulas (θ is the angle between $\mathbf{v}_2$ and $\mathbf{v}_0$):

$$v_0 \approx v_1 - v_2\cos\theta, \tag{11}$$

$$\varepsilon \approx -2m_1v_1v_2\sin\frac{\chi}{2}\cos(\widehat{v_2\nu}) - 2m_1\frac{m_1}{m_2}v_1^2\sin^2\frac{\chi}{2}$$

$$+ 2m_1v_2^2\cos\theta\sin\frac{\chi}{2}\cos(\widehat{v_2\nu}) = \varepsilon_1 + \varepsilon_2. \tag{12}$$

The first of the three terms in formula (12), designated as ϵ_1, is of the order of magnitude $\sqrt{m_1/m_2}E$, and the remaining two terms (ϵ_2) are of order $(m_1/m_2)E$.

We will now perform an expansion in the parameter $\sqrt{m_1/m_2}$ in the right-hand part of (8). The terms of zero order are missing, since in this approximation $f'F' - fF = 0$. The terms of first order fall out on integration. Therefore we will calculate the following nonvanishing terms of order $(m_1/m_2)E$:

$$\mathrm{St}^{(2)} = \int\left\{\left[\frac{\partial f}{\partial E}\varepsilon_2F + \frac{\partial F}{\partial E_2}(-\varepsilon_2)f + \frac{\partial f}{\partial E}\frac{\partial F}{\partial E_2}\varepsilon_1^2\right]v_1\right.$$

$$+\left[\frac{1}{2}\frac{\partial^2 f}{\partial E^2}\varepsilon_1^2F + \frac{1}{2}\frac{\partial^2 F}{\partial E_2^2}\varepsilon_1^2f\right]v_1$$

$$\left.+\left[\frac{\partial f}{\partial E}\varepsilon_1F + \frac{\partial F}{\partial E_2}(-\varepsilon_1)f\right](-v_2\cos\theta)\right\}\frac{\sigma_0}{4\pi}d\mathbf{v}_2do.$$

In order not to complicate the calculations we will omit here terms containing $\partial\sigma/\partial E$, limiting ourselves to the hard-sphere model, for which $\sigma(v, \chi) = \sigma_0/4\pi = \text{const}$; σ_0 is the total cross section, which is the same as the transport cross section. For low electron energies where the scattering is mainly s wave, this model is suitable.

Omitting the intermediate calculations including substitution of Eq. (9) and integration, we write out the result obtained:

$$\frac{\partial f}{\partial t} = \delta\nu E^2T'\frac{\partial}{\partial E}\left[\frac{1}{|E|}\left(\frac{\partial f}{\partial E} + \frac{1}{T'}f\right)\right]. \tag{13}$$

The effective collision frequency is

$$\nu(E) = n_2\sigma_0(2|E|/m_1)^{1/2},$$

$$T' = T\left(1 + \frac{m_2v_i^2}{3T}\right), \quad \delta = 2\frac{m_1}{m_2}.$$

The stationary solution of this equation has the form (E < 0)

$$f(E) = C_1(E - T') + C_2 \exp(-E/T'). \quad (14)$$

The constants C_1 and C_2 are determined by the boundary conditions.[6] One of them is the absorption condition $f(E_0) = 0$ at large negative energy values $|E_0| \gg T'$ (E_0 does not appear in the answer). The other is the condition on the boundary of the regions of finite and infinite motion for $E = 0$. In the region of infinite motion $E > 0$ the electron distribution is of the Maxwell-Boltzmann type:

$$f = (2\pi m_1 T)^{-3/2} \exp\left(-\frac{m_i(\mathbf{v}_1 + \mathbf{v}_i)^2}{2T}\right), \quad (15)$$

where the normalization in momentum space is to $d\mathbf{p}_1$.

For $E = 0$ the distribution of finite electrons must agree with the function (15) averaged over the finite motion:

$$f(E=0) = (2\pi m_1 T)^{-3/2} \exp\left(-\frac{m_1 v_i^2}{2T}\right) \approx (2\pi m_1 T)^{-3/2}. \quad (16)$$

The constants C_1 and C_2 are easily found:

$$C_1 = -\frac{(2\pi m_1 T)^{-3/2}}{T'}, \quad C_2 = -C_1 E_0 \exp(E_0/T'). \quad (17)$$

Equation (13) has the Fokker-Planck form:

$$\partial f/\partial t + A(E)\partial j/\partial E = 0,$$

where j is the particle flux in energy space:

$$j = -B\left(\frac{\partial f}{\partial E} + \frac{1}{T'} f\right). \quad (18)$$

The coefficient A is determined from conservation of the number of particles and, for normalization of the distribution function to one particle, is[6]

$$A = |E|^{5/2}(\sqrt{2}\pi^3 e^6 Z^3 m_1^{3/2})^{-1}.$$

The coefficient B is now determined automatically from Eq. (13):

$$B = 2\pi^3 m_1 \delta e^6 Z^3 T'/l|E|, \quad (19)$$

where $l = (n\sigma_0)^{-1}$ is the electron mean free path.

Calculating the flux j by means of Eqs. (14) and (18), we obtain

$$j(v_i) = -BC_1 \frac{E}{T'} = -\frac{\pi\sqrt{2\pi}}{2} \frac{\delta e^6 Z^3}{m_1^{1/2} l T^{5/2}(1 + m_2 v_i^2/3T)}. \quad (20)$$

The recombination coefficient of a stationary ion α_0 is

$$\alpha_0 = -j(0) = \frac{\pi\sqrt{2\pi}}{2} \frac{\delta e^6 Z^3}{m_1^{1/2} l T^{5/2}}. \quad (21)$$

Averaging the flux (20) over the ionic distribution function (1), we find the recombination coefficient, with inclusion of the thermal motion of the ions:

$$\alpha = 3\left[1 - \left(\frac{3\pi}{2}\right)^{1/2} e^{3/2}(1 - \Phi(\sqrt{3/2}))\right]\alpha_0 \approx 0.56\alpha_0, \quad (22)$$

where

$$\Phi(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

is the probability integral.

We note in conclusion that the coefficient α calculated from formula (22) is close to the Thomson value and roughly six times smaller than that obtained by Pitaevskiĭ. The fact is that in calculating the coefficient B from formula (12) Pitaevskiĭ[6] used Eq. (14), which does not follow from the theory. Bates and Khare[11] have made a numerical calculation of the recombination coefficient of electrons in helium according to the mechanism $He^+ + e + He \rightarrow 2He$ with direct inclusion of the discrete nature of the spectrum for $E < 0$. The result of this calculation, as the authors themselves note, is close to the Thomson value over a substantial range of temperature and density.

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