PHASE SPACE CALCULATION OF THREE BODY ELECTRON-ION RECOMBINATION RATES

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A three body electron ion recombination rate has been calculated using a classical phase space concept. The collision between three particles is represented by a point in phase space, and a distribution of points is assumed corresponding to a gas in thermo-dynamic equilibrium. A "trial" surface separating the free and bound states of the ion-electron pair is chosen at an arbitrary energy below the dissociation limit and the rate at which representative points cross it is calculated. A least upper bound to the recombination rate is obtained by minimizing this crossing rate with respect to the energy level of the "trial" surface. The minimum occurs when the trial surface is at a depth approximately $\frac{5}{2}kT$ below the continuum. Evaluating the rate at the minimum, numerical values are found which agree favourably with other classical results obtained from summing the collisional de-excitation processes.

The rate of recombination of electrion-ion pairs in the presence of an electron is calculated using a classical phase space method previously used to calculate the rate of atom-atom recombinations in the presence of inert gases[1]. The reaction is represented by the equation

$$A^+ + e^- + e^- \rightarrow A + e^-$$

and is known to be important at high electron densities and low temperatures when radiative transitions are unimportant.

In the theory, a three particle collision is represented by the trajectory of a representative point in an eighteen dimensional phase space and is governed by the classical equations of motion. If a "trial" surface is chosen in the phase space, which divides the free and bound states of the electron-ion pair, then a

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necessary condition for a reaction is that a trajectory cross the "trial" surface at least once. For a system in thermodynamic equilibrium the "trial" surface will be crossed an equal number of times from both directions. An upper bound for the recombination rate is calculated by counting all crossings of the "trial" surface in one direction.

Since the theory is classical it can only be justified when the deBroglie wavelength of the electrons is smaller than the characteristic range of the interaction. The appropriate range here is Thomson's radius[2], $2e^2/3kT$, at which the potential energy of the recombining pair is equal to the kinetic energy, and inside which two ions have a high probability of recombining. Based on this radius a classical solution is valid for temperatures below about 11 000° K.

The theory also requires that the Debye length be smaller than the mean free path, but larger than the Thomson radius. The first condition insures that the three body collisions are independent and the second that the potentials will not be screened in the interaction zone. For electron temperatures of 1 000° K and 10 000° K these conditions will be satisfied providing the electron density does not exceed 10^{16} and 10^{19} cm^{-3}, respectively.

The "trial" surface chosen for the present calculation is defined by the condition that the relative energy of the recombining electron-ion pair be $-E_c$ with respect to the dissociation limit. It is shown schematically in fig. 1 along with a diagram of the three particle system. The rate at which representative points cross this "trial" surface is[1]

$$R = \int \rho_0 \exp\{-H/kT\}\, v\cdot n \, d\sigma \tag{1}$$

where $v\cdot n$ is the normal velocity with respect to an element of surface $d\sigma$, H is the total Hamilitonian for the three bodies and ρ_0 is a constant. In the center of mass system, the flux integral is 11 dimensional and the integration is carried out keeping $\varepsilon_c = E_c/kT$) as an undetermined parameter. Coulomb potential fields are assumed between each pair of particles and the three body potential is assumed to be the sum of two body potentials. The three body recombination rate constant is then given by

$$k = R/n_1 n_e^2 = 2\pi^{\frac{1}{2}}\left(\frac{8\,kT}{\pi m}\right)^{\frac{1}{2}} r_T^5 \exp\{\varepsilon_c\}\, \Gamma(\varepsilon_c) \tag{2}$$

where

$$\Gamma(\varepsilon_c) = \int \exp\{-(\varepsilon_3+u_3)\}\frac{1}{\rho_{23}^2}\left(\frac{1}{\rho_{12}}-\varepsilon_c\right)\varepsilon_3^{\frac{1}{2}}\, d\varepsilon_3\, \rho_{12}^2\, d\rho_{12}\, \rho_{13}^2\, d\rho_{13}\, d\cos\theta\, d\cos\gamma \tag{3}$$

and $r_T = e^2/kT$, $\rho_{13} = r_{13}/r_T$, $\rho_{23} = r_{23}/r_T$, $\rho_{12} = r_{12}/r_T$, $\varepsilon_3 = mv_3^2/2kT$,

v_3 is the velocity of particle 3 and $u_3 = 1/\rho_{23} - 1/\rho_{13}$ is the sum of the potentials between particle 1 − 3 and 2 − 3 divided by kT. Other symbols are defined in fig. 1. The integration of eq. (3) is to be carried out subject to the conditions $v \cdot n \geq 0$, $H_{12} = (-E_c)$ and $H_{13} \geq (-E_c)$ where H_{12} and H_{13} are the relative energies of the two electrons with respect to the ion. The last condition is imposed to insure that one electron has not already crossed the "trial" surface and hence recombined with the ion.

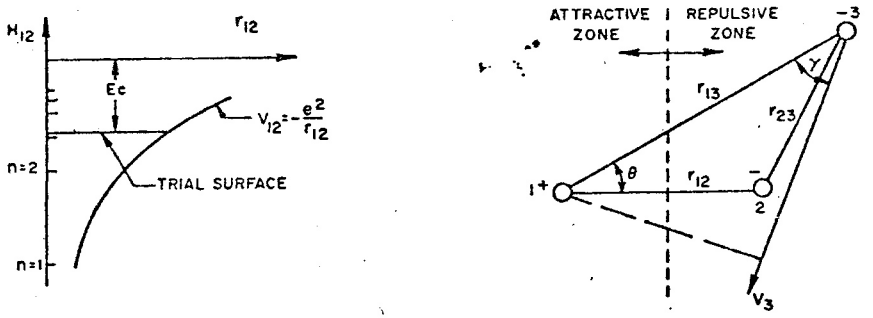

Fig. 1. Schematic diagram showing location of "trial surface separating "free" and "bound" states of an electron-ion pair and geometry of the three body collision.

As it stands the integral in eq. (3) diverges linearly in ρ_{13}. Such divergences are well known with Coulomb potentials and are the result of many long range "soft" collisions. The "trial" surface may be crossed many times by a single point during such collisions resulting in a gross overestimate of the net recombination rate. However, in collisions of this type, no energy is transferred between the particles and recombination will not occur. Bohr[3] showed that when the product of the collision time (τ) and the angular frequency of a bound electron round its parent nucleus (ω) is greater than unity the collision is adiabatic and no energy will be transferred. Since we are only interested in those collisions where energy is transferred, we may limit the integral in eq. (3) to the region where $\omega\tau \leq a$, where a is a cut-off parameter of order unity. The integration may then be carried out approximately[4] and the result expressed in the form

$$\Gamma(\varepsilon_c) = \Gamma_a(\varepsilon_c) + \Gamma_r(\varepsilon_c) \tag{4}$$

where

$$\Gamma_a(\varepsilon_c) = \frac{3a^2}{64\sqrt{\pi}}\left[8\exp\left\{\tfrac{3}{5}\varepsilon_c\right\} - 3\right]\varepsilon_c^{-4} \tag{5}$$

and

$$\Gamma_r(\varepsilon_c) = \frac{3a^2}{16\sqrt{\pi}}\varepsilon_c^{-4} \tag{6}$$

are the contributions to $\Gamma(\varepsilon_c)$ from the zones in which the potential of the "third body" electron is attractive and repulsive, respectively.

As can be seen from eq. (2) the rate at which trajectories cross the "trial" surface depends on the factor $\Gamma(\varepsilon_c)\exp(\varepsilon_c)$ which is shown plotted in fig. 2. This factor has a minimum value at $\varepsilon_c = \frac{5}{2}$ giving a three body recombination rate constant

$$k = 2.3 \times 10^{-8} a^2 T^{-\frac{9}{2}}. \tag{7}$$

This minimum or "bottleneck" in the equilibrium crossing rate is a simple consequence of the fact that as the energy level of the "trial" surface in-

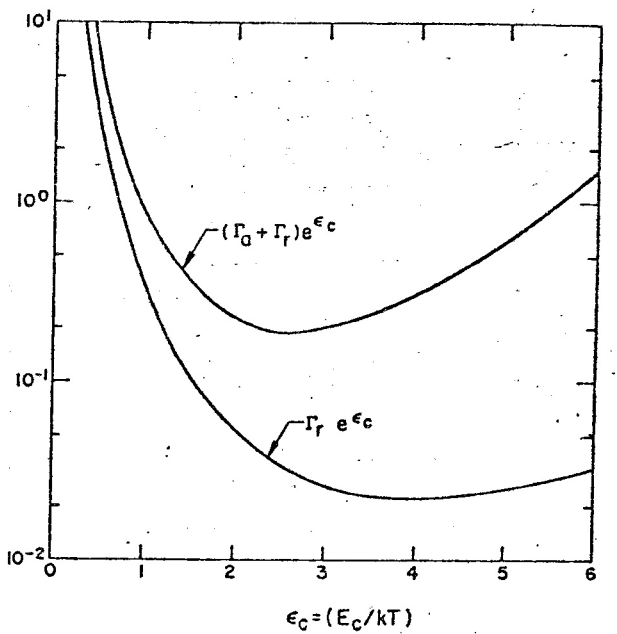

Fig. 2. Plot of the factors $(\Gamma_a + \Gamma_r)\exp(\varepsilon_c)$ and $\Gamma_r \exp(\varepsilon_c)$ giving the dependence of the total crossing rate and the crossing rate for repulsive collisions on the level of the "trial" surface.

creases, probability of collisional transitions $\Gamma(\varepsilon_c)$ increases while the equilibrium density exp (ε_c) decreases.

Also shown in fig. 2 is the factor $\Gamma_1(\varepsilon)$ exp (ε_c) which gives the partial contribution to the rate from the zone in which the interaction with the "third body" electron is repulsive. At the location of the "bottleneck" in $\Gamma(\varepsilon_c)$ exp (ε_c) at $\varepsilon_c = \frac{5}{2}$ this factor contributes less than 20% of the total rate showing that attractive collisions are much more important than repulsive.

The rate constant given by eq. (7) for several values of the cut-off parameter a is compared with that calculated by Bates, Kingston and McWhirter[5] in fig. 3 and the agreement is surprisingly good considering the wide divergence in the methods used. Bates *et al.* considered the problem from the point of view of cascading between levels using transition probabilities obtained by Gryzinski[6] from a classical treatment of an equivalent two body problem in which the influence of the ion is neglected except for its effect on the momentum distribution of the bound electron. The problem has also been treated by Byron, Stabler and Bortz[7] who used Gryzinski's transition probabilities and whose results agree with those of Bates *et al.*. Byron *et al.* found a "bottleneck" in the equilibrium transition rate at approximately

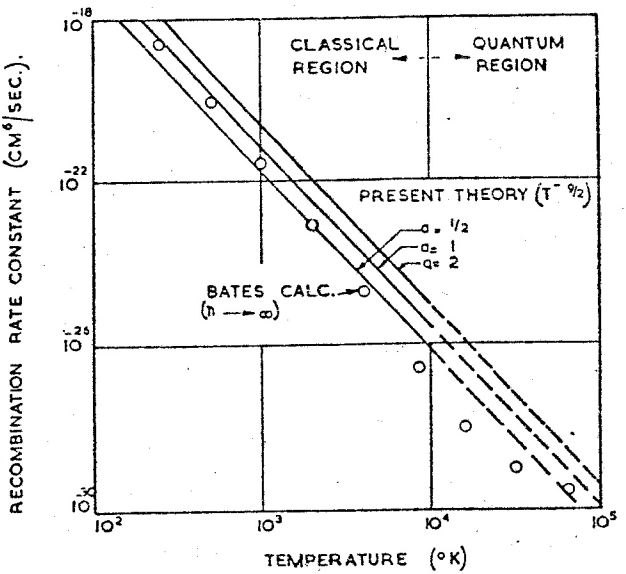

Fig. 3. Comparison of present results with those calculated by Bates for infinite electron density using Gryzinski's classical transition probabilities. Note that the extension of either Bates' OR the present results into the quantum mechanical region is of doubtful validity.

3 kT below the dissociation limit which is close to the value of $\frac{5}{2}$ kT determined in the present calculations.

The existence of a "bottleneck" in the de-excitation rate has been observed experimentally by Hinnov and Hirschberg[8] who measured the population of states in a recombining helium plasma. Their results are shown in fig. 4 where we have plotted the ratio of the observed populations to those expected of equilibrium as a function of the parameter E_n/kT where E_n is the

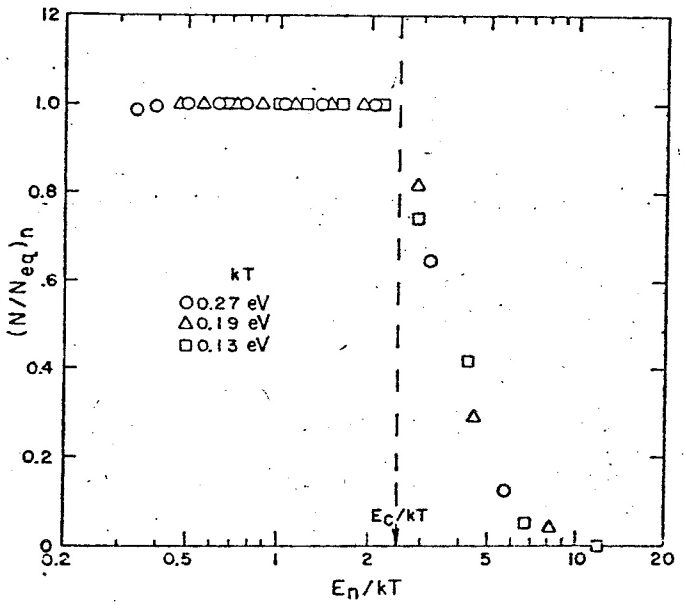

Fig. 4. Plot of the population distributions observed by Hinnov and Hirschberg for a recombining helium plasma showing departure from equilibrium at approximately $\frac{5}{2}$ kT below the dissociation limit as predicted by the theory. In effect this reduces the ionization potential by this amount.

energy of the n^{th} quantum level below the dissociation limit. When plotted in this manner, the observations at different temperatures all fall on a single curve which drops sharply from unity in the neighborhood of $E_n/kT = \frac{5}{2}$ as predicted by the theory.

An important effect which is taken into account in the present calculation which is neglected in Gryzinski's work is the influence of the ionic charge on the motion of the "third body" electron. The magnitude of this effect may be judged from fig. 2 which shows that over 80% of the calculated recombination rate comes from the region in which the net interaction with the "third body" electron is attractive. A further improvement on Gryzinski's calculation is in

the treatment of the "adiabatic" collisions which Gryzinski eliminated by an arbitrary averaging procedure.

In concluding we should like to point out that although the theory presented here does not give results which are startling different from those of Bates *et al.* and Byron *et al.* they were obtained by a simpler and more direct method which is capable of giving an insight into the specifically three body effects and can be subject to systematic improvement.

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