THE THERMODYNAMICS OF A DENSE PLASMA

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The classical equations of motion of a system consisting of a small number of electrons and ions are integrated numerically assuming that at a distance $r = r_i$ between an electron and an ion the electron is elastically reflected from the ion. We show that when $r_i \approx 0.5 \times 10^{-8}$ cm the potential energy of the Coulomb interaction Π and the plasma pressure on the wall p, evaluated from the momentum transferred to the wall in elastic collisions are the same as those given by the Debye approximation in a range of values of T and n (T—temperature and n—electron concentration) for which the total energy of the plasma E is positive. This region is bounded from below in the T-n plane by the curve $T = T_0 (n/n_0)^{1/3}$, $T_0 = 13800^\circ$K, $n_0 = 2 \times 10^{20}$ cm^{-3}, along which the pressure of a Coulomb plasma is less than the pressure of an ideal plasma ($p_{id} = 2nkT$) for the same parameters by a factor two. We find the mean free path l in a dense plasma which turns out to be an order of magnitude smaller than the value of l given by the formula containing the "Coulomb logarithm."

IN the present paper we make an attempt to obtain the thermodynamic quantities for a dense plasma by considering microscopic volumes of the plasma (microplasma), containing 10 to 100 particles.

The number of particles of a microplasma, needed to obtain correct values of the macroscopic quantities, depends on the plasma density and its temperature. As a qualitative a priori estimate we can use the number of particles N_d in a Debye sphere, calculated in the Debye approximation. If for some values of the parameters n and T, where n is the electron concentration and T the temperature, N_d is small, e.g., $N_d \lesssim 1$ (using the formula for the radius of the Debye sphere one checks easily that, for instance, for $n = 2 \times 10^{20}$ cm^{-3}, $T = 15\,000^\circ$K the number of particles $N_d \ll 1$) we can try to predict the properties of a plasma by a system consisting, for instance, of 50 electrons and 50 ions. The preliminary estimates of N_d can, of course, not be considered a priori to be correct. It is thus necessary when evaluating the properties of the microplasma to calculate the radius d of the Debye sphere and also the mean free path l. If the values of d and l found numerically turn out for some values of the parameters n and T to be less than the linear dimensions a_0 of the microplasma, then we can attribute the thermodynamic quantities found in the calculating process to a macroscopic plasma volume with the same parameters.

It is natural that the number of particles of the microplasma must preferably be chosen as large as possible so that the mean square fluctuations of the physical quantities are diminished, but increasing the number of particles is hindered by the limited possibilities of electronic computers.

The equations of motion of a system consisting of N electrons and N ions with a Coulomb interaction have in dimensionless variables the form (in the system of 2N particles, the electrons are numbered from 1 to N, and the ions from N + 1 to 2N):

$$\dot{x}_{i\alpha} = u_{i\alpha} \quad (\alpha = 1, 2, \ldots, 2N), \tag{1}$$

$$\dot{u}_{i\alpha} = F_0\left\{-\sum_{\beta\neq\alpha=1}^{N}\frac{x_{i\beta}-x_{i\alpha}}{r_{\alpha\beta}^3}+\sum_{\beta=N+1}^{2N}\frac{x_{i\beta}-x_{i\alpha}}{r_{\alpha\beta}^3}\right\} \quad (\alpha = 1, 2, \ldots N), \tag{2}$$

$$\dot{u}_{i\alpha} = -\frac{m}{M}F_0\left\{-\sum_{\beta=1}^{N}\frac{x_{i\beta}-x_{i\alpha}}{r_{\alpha\beta}^3}+\sum_{\beta\neq\alpha=N+1}^{2N}\frac{x_{i\beta}-x_{i\alpha}}{r_{\alpha\beta}^3}\right\}$$
$$(\alpha = N+1, \ldots, 2N),$$
$$r_{\alpha\beta} = \left[\sum_{k=1}^{3}(x_{k\beta}-x_{k\alpha})^2\right]^{1/2}, \tag{3}$$
$$F_0 = e^2/a_0 m v_0^2 = \Pi_0/2K_0,$$

where $x_{i\alpha}$ and $u_{i\alpha}$ (i = 1, 2, 3) are dimensionless Cartesian coordinates and velocity components of the α-th particle; $r_{\alpha\beta}$ is the distance between particles α and β; m the electron and M the ion mass; we assume that the ions are singly ionized; a_0 is a unit of length which is equal to the edge of the cube in which the microplasma is contained; v_0 is a unit of velocity (depending on the magnitude of v_0 the kinetic energy of the system is changed and hence also the plasma temperature); $\Pi_0 = e^2/a_0$ is the unit of potential energy; $K_0 = mv_0^2/2$ is the unit of the kinetic energy; $\tau_0 = a_0/v_0$ is the unit of time.

It is well known from statistical physics[1] that the thermodynamic potentials of a system with Coulomb interactions depends on one function of one variable. From an analysis of the properties of the partition function[1] or of the set of equations (1)–(3) it follows that the following transformation is valid:

$$T' = \gamma T, \quad n' = \gamma^3 n, \quad \Pi' = \gamma\Pi, \tag{4}$$

i.e., multiplying T by γ and n by γ^3 leads to multiplying the potential energy of the Coulomb interaction Π by γ. The transformation (4) makes it possible to construct Π as a function of n and T if the potential energy Π_0 for some single value n_0 of the concentration is known as a function of T:

$$\Pi(n, T) = (n/n_0)^{1/3}\Pi_0(T(n_0/n)^{1/3}). \tag{5}$$

We note that the potential energy Π_1 of the plasma for one electron-ion pair in the Debye approximation,[2,3]

$$\Pi_1 = -\sqrt{8\pi}e^3\sqrt{n/kT} \tag{6}$$

satisfies the transformation (4).

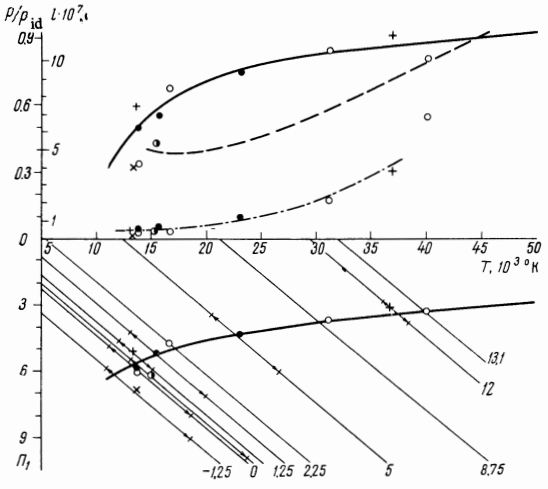

FIG. 2. The T-dependence of Π_1, p/p_{id}, and l (the scale for Π_1 and E_1 is 10^{-12} erg).

ticle. From the magnitude of K_1 we determined the plasma temperature using the formula $K_1 = {}^3/_2\,kT$. The Debye screening radius was determined from the relation $d = e^2/\Pi_1$ or

$$d / a_0 = \Pi_0 / \Pi_1. \qquad (12)$$

In the lower part of Fig. 2 the full-drawn line gives the T-dependence of Π_1 for $n = 2.10^{20}$ cm^{-3} evaluated in the Debye approximation using Eq. (6). The parallel lines at an angle to the T-axis correspond to the lines E = const. (The equation of these lines is $\Pi_1 = -3kT + E_1$.) The numbers standing near each line correspond to the values of E_1 for which the values of Π_1 were evaluated numerically.

In the upper part of Fig. 2 the full-drawn curve gives p/p_{id} found from Eq. (8) in the Debye approximation. (The curves for Π_1 and p/p_{id} are given down to a temperature $T \approx 11\,000^\circ$K below which the stability condition $(\partial p/\partial V)_T < 0$ is violated.) The dashed line indicates the T-dependence of l for Coulomb collisions, evaluated from the formula [4]

$$l = \frac{9}{4\pi}\frac{(kT)^2}{ne^4\lambda}, \quad \lambda = \ln\left(\sqrt{\frac{9\pi}{32}}\frac{(kT)^{3/2}}{e^3 n^{1/2}}\right) \qquad (13)$$

($n = 2 \times 10^{20}$ cm^{-3}). The dot-dash line is drawn through points corresponding to numerically obtained values of l. Slanted crosses and black dots indicate numerically obtained values of Π_1, p/p_{id}, and l for a system with N = 64 and for $r_i = 0.5 \times 10^{-8}$ cm, the crosses for $r_i = 1.5 \times 10^{-8}$ cm, and the black-white points for $r_i = 0.3 \times 10^{-8}$ cm. The circles indicate the values of the same quantities for a system with N = 16, $r_i = 0.43 \times 10^{-8}$ cm. The range of oscillations in Π_1 occurring in the numerical integration is indicated by the arrows drawn along the lines E_1 = const (for N = 64).

It can be seen from Fig. 2 that for $r_i \approx 0.5 \times 10^{-8}$ cm the numerically obtained values for Π_1 and p/p_{id} are close to the values given by the Debye approximation, provided the total energy is non-negative, $E_1 \geq 0$. In the region of negative values of E_1 there occurs a steep deviation of the calculated values of Π_1 and p/p_{id} from the theoretical curves. For $r_i = 1.5 \times 10^{-8}$ cm the calculated values of Π_1 and p/p_{id} lie above, and for $r_i = 0.3 \times 10^{-8}$ cm below the theoretical curves by approximately 10–15%.

The numerically obtained values of l are less than the values of l given by Eq. (13) by approximately an order of magnitude in the whole range of energies E_1 studied. This shows that Eq. (13) for the "Coulomb logarithm" λ can not be assumed to be correct in the range of values of T and n for which $E_1 < 10^{-11}$ erg.

We note that the transformation (4) applied both to (11) and to (13) leads to a decrease in l by a factor γ. Similarly, the transformation (4) applied both to (12) and to the equation

$$d = (kT / 8\pi ne^2)^{1/2}, \qquad (14)$$

leads to a decrease in the Debye radius by a factor γ.

In the table we have given values of l/a_0 and d/a_0 obtained when computing the properties of an electron-positron plasma in its dependence on E_1 (or T). We have also given the dimensionless time h of integration over a section in thermodynamic equilibrium, the total number of distant, Σf_d, and close, Σf_c, collisions and also the number of collisions of particles with the wall, f_w. It can be seen from the table that the numerically obtained values of l/a_0 and d/a_0 are simultaneously less than unity for all $E_1 < 10^{-11}$ erg. Hence we may assume that the requirements imposed upon the number of particles in the microplasma are satisfied in the range $E_1 < 10^{-11}$ erg.

For an ion radius $r_i \approx 0.5 \times 10^{-8}$ cm the numerically obtained values of Π_1 are thus close to the values given by plasma theory in the Debye approximation; taking also into account that the Debye approximation is valid for a plasma which differs little from an ideal one, $\Pi_1 \lesssim 0$ we can state that (for $r_i = 0.5 \times 10^{-8}$ cm) the thermodynamics of the plasma in the Debye approximation is applicable to the whole range $E_1 \geq 0$. In the T, n plane this region is bounded from below, as follows from the transformation (4) by the curve $T = T_0(n/n_0)^{1/3}$, $T_0 = 13\,800^\circ$K, $n_0 = 2 \times 10^{20}$ cm^{-3} along which $E_1 = 0$, and along which, according to the virial theorem, the plasma pressure is smaller than the pressure of the ideal

N	64							16			
$r_i \cdot 10^8$, cm	0,5				0,3	1,5		0,43			
$E_1 \cdot 10^{12}$, erg	−1.25	−0.2	1.25	5	0	0.3	12	−0.2	2.25	8.75	13.1
T, °K	13 600	13 800	15 400	22 800	15 200	13 400	36 600	13 900	16 700	31 000	40 000
h	0.36	0.45	0.71	0.53	0.21	0.63	0.62	0.64	0.34	0.44	0.51
l/a_0	0.028	0.078	0.10	0.18	0.079	0.05	0.61	0.063	0.15	0.52	1.4
d/a_0	0.045	0.064	0.065	0.077	0.054	0.065	0.11	0.09	0.11	0.14	0.16
Σf_d	562	656	600	339	267	441	107	155	39	11	8
Σf_c	1100	208	254	170	122	1200	142	72	14	16	2
f_w	30	53	100	108	20	96	150	15	20	33	35

Thanks to (4) the problem of obtaining the thermodynamic potentials with an electronic computer is greatly simplified since it is sufficient to determine the potential energy as function of the temperature for one arbitrary value of the electron concentration. Once the value of Π is found one can easily obtain the thermodynamic potentials of the plasma through well-known formulae[1]. The equation of state of the plasma can be obtained by using the virial theorem for a system with Coulomb interactions:[1]

$$pV = (K+E)/3, \tag{7}$$

where p is the pressure, V the volume of the system, E = Π + K the total energy and K the kinetic energy of the system.

One can write Eq. (7) in the form

$$p/p_{id} = 1 + \Pi_1/6kT, \quad p_{id} = 2nkT. \tag{8}$$

We integrated Eqs. (1)—(3) on the M-20 computer by a fourth order Runge-Kutta method. The criterion for the exactness (and validity) of the integration was the energy conservation law, E = const. The initial values of the coordinates $x_{i\alpha}$ and the velocities $u_{i\alpha}$ were given from a random number data unit, uniformly distributed for the coordinates in the interval 0 to 1 and for the velocities in the interval ±(0.66 to 1). For some variants we chose for the initial values of $x_{i\alpha}$ and $u_{i\alpha}$ finite values of the same quantities from some other variant where all velocities might be multiplied by some constant changing thereby the magnitude of the kinetic energy according to our own wishes.

The concentration of the electrons n_0 was in all cases equal to 2×10^{20} cm^{-3}. The calculation was performed for an electron-positron plasma (in that case we must in (3) take M = m) with the electron number N = 16, $a_0 = (N/n_0)^{1/3} = 0.43 \times 10^{-6}$ cm and N = 64, $a_0 = 0.685 \times 10^{-6}$ cm.

The choice made of an electron-positron plasma as compared to a more natural electron-ion plasma is explained by the fact that the time to reach the thermodynamic equilibrium regime (relaxation time) is by far smaller for an electron-positron plasma than for an electron-ion one. And as the thermodynamic quantities are independent of the particle masses (provided we are not interested in relaxation times) the consideration of an electron-positron plasma considerably shortens the machine calculating time.

When integrating the set of equations we evaluated after each step in the integration the following quantities:

a) The interaction potential energy

$$\Pi = \Pi_0 \left\{ \sum_{\alpha=1}^{N} \sum_{\beta>\alpha}^{N} \frac{1}{r_{\alpha\beta}} + \sum_{\alpha=N+1}^{2N} \sum_{\beta>\alpha}^{2N} \frac{1}{r_{\alpha\beta}} - \sum_{\alpha=1}^{N} \sum_{\beta=N+1}^{2N} \frac{1}{r_{\alpha\beta}} \right\}. \tag{9}$$

b) The kinetic energy of the electrons, K_e, of the positrons, K_p, and of each particle, K_α, separately.

c) The total energy of the system E = Π + K_e + K_p.

d) The momentum transferred by the particles to the wall in elastic collisions through which the pressure of the plasma on the wall is immediately defined:

$$p = p_0(u_\perp/h), \tag{10}$$

where $p_0 = 2mv_0^2/6a_0^3$, $h = \Delta t/\tau_0$ is the total dimensionless time of integration over an interval in thermodynamic equilibrium, $u_\perp$ the sum of the components at right angles to the wall of the velocities of the particles which collide with the walls in a time interval Δt.

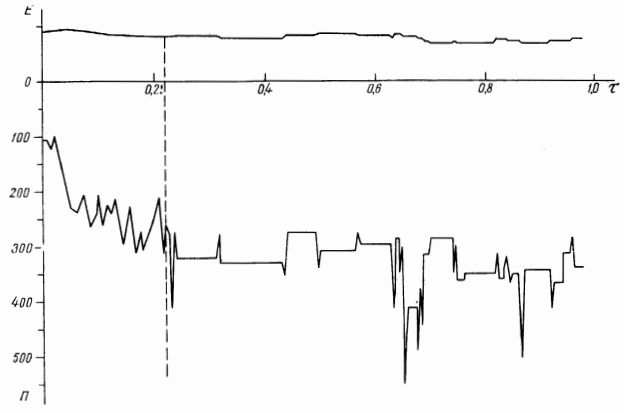

FIG. 1. The τ-dependence of Π and E (the scale along the vertical axis is 10^{-12} erg, and along the horizontal axis 10^{-14} sec).

e) The number of distant collisions f_d; we assumed here that a particle has undergone a distant collision if as a result of interactions it has accumulated a change in the direction of its velocity over an angle larger than π/2.

f) The number of close collisions f_c; we assumed here that an electron α underwent a close collision, if first of all it found itself at a distance $r_{\alpha\beta} \leq r_i$ from some positron β; and secondly the direction of the velocity u_α of the electron was forced to change by an angle equal to π in order that a closer approach of the electron α to the positron β be avoided. This procedure corresponds to an assumption that for $r_{\alpha\beta} = r_i$ (ion radius) the electron is reflected from the ion retaining its energy.

From the number of collisions f undergone by one particle during a time h we calculated the mean free path:

$$l/a_0 = \mu h/f, \tag{11}$$

where μ is the dimensionless mean velocity of the particles.

In Fig. 1 we have given the curve showing the variation in time of the potential energy Π obtained as a result of numerically integrating for the variant with energy E_1 per electron-positron pair of 1.25×10^{-12} erg, N = 64. (The sections parallel to the τ-axis show parts of the curve, on which the oscillations in the potential energy did not exceed some value ΔΠ, averaged over the time.) In the same figure we have given the curve giving the change in the total energy E of the system. It can be seen that the total energy does not stay exactly constant due to inexact integration. However, the deviation of E from its average value is small compared to Π and has a magnitude $< 5\%$.

The graphs given in Fig. 1 are typical also for other variants with different values of E_1 and N. From these curves we determined along those sections which correspond to the thermodynamic equilibrium state (in Fig. 1 to the right of the vertical dotted line) the time average of the potential energy Π_1 per electron-positron pair and the average value of the kinetic energy K_1 per par-

plasma by a factor two. For $r_i = 1.5 \times 10^{-8}$ cm we must in Eq. (6) for Π_1 in the range $0 < E_1 < 10^{-11}$ erg introduce a coefficient ≈ 0.9 and for $r_i = 0.3 \times 10^{-8}$ cm a coefficient ≈ 1.1.

The numerical values of r_i met with in this paper are correct for $n_0 = 2 \times 10^{20}$ cm^{-3}. When changing to other concentrations we must also apply to r_i the transformation (4) which leads to decreasing r_i by a factor γ.

[1] L. D. Landau and E. M. Lifshitz, Statisticheskaya fizika (Statistical Physics), Nauka, 1964, p. 1964 (English translation published by Pergamon Press, 1968).

[2] D. A. Frank-Kamenetskiĭ, Lektsii po fizike plazmy (Lectures on Plasma Physics), Atomizdat, 1964, p. 53.

[3] A. A. Vedenov, in the collection Voprosy teorii plazmy (Plasma Theory Problems) 1, 273 (1963) (English translation published under the title Reviews of Plasma Physics, Vol. 1, by Consultants Bureau, 1965).

[4] B. A. Trubnikov, in the collection Voprosy teorii plazmy (Plasma Theory Problems) 1, 98 (1963) (English translation published under the title Reviews of Plasma Physics, Vol. 1, by Consultants Bureau, 1965).

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