APPROXIMATIONS OF "FREE" AND "BOUND" CHARGES FOR A SYSTEM OF CHARGED PARTICLES. SELF-CONSISTENT EQUATIONS FOR SECOND DISTRIBUTION FUNCTIONS

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Abstract

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APPROXIMATIONS OF "FREE"AND "BOUND" CHARGES FOR A SYSTEM OF CHARGED PARTICLES. SELF-CONSISTENT EQUATIONS FOR SECOND DISTRIBUTION FUNCTIONS

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In deriving kinetic equations for a plasma, the assumption that the correlation functions are small is used ([1,2]). In the zeroth approximation one obtains a self-consistent system of equations for the first distribution functions and the mean fields—the system of Vlasov equations. This corresponds to the approximation of "free" charges, since the correlation functions are equal to zero. In the next approximation (in obtaining the collision integral) correlations are taken into account but are assumed to be small. Such an approximation is justified for a fully ionized rarefied plasma. However, it is not entirely satisfactory for the case of a weakly ionized plasma, for example a hydrogen plasma, when each electron spends most of its time near an ion. In the present article equations are considered which describe both the approximation of "free" and of "bound" charges.

The question of taking "bound" charges into account has been considered in connection with the statistical justification of Maxwell' s equations (see, for example, ([3,4])). This question is set out most consistently in the work of Mazur ([4]).

For simplicity we consider here a hydrogen plasma. More general cases may be considered in an analogous way.

Let $a = 1, 2$ be the component index: 1—ions, 2—electrons; $\mathbf{x}_{ai} = (\mathbf{q}_{ai}, \mathbf{p}_{ai})$ is a six-dimensional vector characterizing the state of the i-th particle of component a; $1 \leq i \leq N$; $N_1 = N_2 = N$; $e_1 = |e_2|$.

If electrons and ions are combined into pairs, then the Liouville equation for the distribution function of all particles of the system $f_{2N}(\dots \mathbf{x}_{1i} \dots, \dots \mathbf{x}_{2i} \dots, \dots, t)$ in the case of a Coulomb plasma can be written in the form

$$\frac{\partial f_{2N}}{\partial t} + \sum_{1\le i<N,\ a} \left\{ \mathbf{v}_{ai} \frac{\partial f_{2N}}{\partial \mathbf{q}_{ai}} - \frac{\partial \Phi(|\mathbf{q}_{ai} - \mathbf{q}_{bi}|)}{\partial \mathbf{q}_{ai}} \frac{\partial f_{2N}}{\partial \mathbf{p}_{ai}} - e_a \frac{\partial U(\mathbf{q}_{ai})}{\partial \mathbf{q}_{ai}} \frac{\partial f_{2N}}{\partial \mathbf{p}_{ai}} \right\} = 0, \tag{1}$$

$$b \neq a = 1, 2.$$

Here Φ is the Coulomb potential energy of a pair. The potential is determined by the equation

$$\frac{\partial^2 U}{\partial \mathbf{q}_{ai}^2} = -4\pi e_1 \sum_{1\le j<N} \left[\delta(\mathbf{q}_{ai} - \mathbf{q}_{1j}) - \delta(\mathbf{q}_{ai} - \mathbf{q}_{2j}) \right], \quad j \neq i \text{ for } a = 1 \text{ or } a = 2. \tag{2}$$

Instead of the system of equations (1), (2), one may take as the starting point the equation for the microscopic potential U and the phase density in the space $\mathbf{q}_a, \mathbf{q}_b, \mathbf{p}_a, \mathbf{p}_b$ $(a, b = 1, 2;\ a \neq b)$

$$N_{ab}(\mathbf{q}_a, \mathbf{q}_b, \mathbf{p}_a, \mathbf{p}_b, t) = \sum_{1\le i<N} \delta(\mathbf{q}_a - \mathbf{q}_{1i}) \delta(\mathbf{q}_b - \mathbf{q}_{2i}) \delta(\mathbf{p}_a - \mathbf{p}_{1i}) \delta(\mathbf{p}_b - \mathbf{p}_{2i}). \tag{3}$$

Neglecting unity in comparison with N, we obtain for the functions N_{ab}, U the equations

$$\frac{\partial N_{ab}}{\partial t} + \mathbf{v}_a \frac{\partial N_{ab}}{\partial \mathbf{q}_a} + \mathbf{v}_b \frac{\partial N_{ab}}{\partial \mathbf{q}_b} - \frac{\partial \Phi(|\mathbf{q}_a - \mathbf{q}_b|)}{\partial \mathbf{q}_a} \frac{\partial N_{ab}}{\partial \mathbf{p}_a} - \frac{\partial \Phi(|\mathbf{q}_a - \mathbf{q}_b|)}{\partial \mathbf{q}_b} \frac{\partial N_{ab}}{\partial \mathbf{p}_b}$$
$$- e_a \frac{\partial U(\mathbf{q}_a)}{\partial \mathbf{q}_a} \frac{\partial N_{ab}}{\partial \mathbf{p}_a} - e_b \frac{\partial U(\mathbf{q}_b)}{\partial \mathbf{q}_b} \frac{\partial N_{ab}}{\partial \mathbf{p}_b} = 0, \tag{4}$$

$$\frac{\partial^2 U}{\partial \mathbf{q}^2} = -4\pi \int \left[e_a \delta(\mathbf{q} - \mathbf{q}_a) + e_b \delta(\mathbf{q} - \mathbf{q}_b) \right] \times$$
$$\times N_{ab}(\mathbf{q}_a, \mathbf{q}_b, \mathbf{p}_a, \mathbf{p}_b, t)\, d\mathbf{q}_a d\mathbf{q}_b d\mathbf{p}_a d\mathbf{p}_b. \tag{5}$$

In the approximation of "free" charges it is convenient to use, as the starting point, the simpler microscopic equations for phase densities in six-dimensional space ([2])

$$N_a(\mathbf{q}, \mathbf{p}, t) = \int N_{ab}\, d\mathbf{q}_b d\mathbf{p}_b = \sum_{1\le i\le N} \delta(\mathbf{q} - \mathbf{q}_{ai}(t))\, \delta(\mathbf{p} - \mathbf{p}_{ai}(t)), \tag{6}$$

$$\frac{\partial N_a}{\partial t} + \mathbf{v}\frac{\partial N_a}{\partial \mathbf{q}} + e_a E(\mathbf{q},t)\frac{\partial N_a}{\partial \mathbf{p}} = 0, \qquad \operatorname{div} E(\mathbf{q},t) = 4\pi \sum_a e_a \int N_a \, d\mathbf{p}. \quad (7)$$

These equations follow from (4), (5).

In the approximation of "bound" charges we use the variables

$$\mathbf{R} = \frac{m_1\mathbf{q}_1 + m_2\mathbf{q}_2}{m_1 + m_2}, \qquad \mathbf{r} = \mathbf{q}_1 - \mathbf{q}_2, \qquad \equiv M\mathbf{V} = \mathbf{p}_1 + \mathbf{p}_2;$$

$$\mathbf{p} \equiv \mu\mathbf{v} = \frac{m_1 m_2}{m_1 + m_2}(\mathbf{v}_1 - \mathbf{v}_2).$$

From (4), for the functions $N_{ab}(\mathbf{R}, \ , \mathbf{r}, \mathbf{p}, t)$ we obtain the equations

$$\frac{\partial N_{ab}}{\partial t} + \mathbf{V}\frac{\partial N_{ab}}{\partial \mathbf{R}} + \mathbf{v}\frac{\partial N_{ab}}{\partial \mathbf{r}} - \frac{\partial \Phi(|\mathbf{r}|)}{\partial \mathbf{r}}\frac{\partial N_{ab}}{\partial \mathbf{p}} - e_1\frac{\partial U^{(-)}}{\partial \mathbf{R}}\frac{\partial N_{ab}}{\partial} - e_1\frac{\partial U^{(-)}}{\partial \mathbf{r}}\frac{\partial N_{ab}}{\partial \mathbf{p}} = 0,$$

$$a = 1, \ b = 2. \quad (8)$$

Here

$$U^{(-)}(\mathbf{R}, \mathbf{r}) = U\left(\mathbf{R} + \frac{m_2}{m_1 + m_2}\mathbf{r}\right) - U\left(\mathbf{R} - \frac{m_1}{m_1 + m_2}\mathbf{r}\right), \quad (9)$$

$$\frac{\partial^2 U}{\partial \mathbf{q}^2} = -4\pi e_1 \int \left[\delta\left(\mathbf{q} - \left(\mathbf{R} + \frac{m_2}{m_1 + m_2}\mathbf{r}\right)\right) - \delta\left(\mathbf{q} - \left(\mathbf{R} - \frac{m_1}{m_1 + m_2}\mathbf{r}\right)\right)\right] \times$$

$$\times N_{ab}(\mathbf{R}, \ , \mathbf{r}, \mathbf{p}, t)\, d\mathbf{R}\, d \ d\mathbf{r}\, d\mathbf{p}. \quad (10)$$

The systems of microscopic equations presented are equivalent. The advantage of one or another form of notation appears upon passing, after averaging, to approximate equations for the lower moments of the random functions N_{ab}, U. Thus, for system (7), the approximation of the first moments corresponds to the self-consistent approximation for the first distribution functions $f_a = \overline{N}_a/n_a$ and the mean field ([2]) (the Vlasov equations).

The approximation of the first moments for system (8) corresponds to the self-consistent approximation for the second distribution function $f_{ab} = \overline{N}_{ab}/n$ ($n_a = n_b = n$) and the mean field created by all particles surrounding the distinguished pair. The equations for the functions $f_{ab}, \overline{U}$ coincide with (8)–

(10) if in them $N_{ab} \to n f_{ab}$, $U \to \overline{U}$. In contrast to the usual self-consistent approximation, the mean field now depends on the correlation function g of pairs of charged particles

$$g(\mathbf{R}, \mathbf{r}, \ , \mathbf{p}, t) = f_{ab}(\mathbf{R}, \mathbf{r}, \ , \mathbf{p}, t) - f_a \cdot f_b. \tag{11}$$

If the distance r, on the average, is considerably greater than the radius of action, then correlations may be neglected and the system of equations for the functions $f_{ab}, \overline{U}$ reduces to the usual system of self-consistent equations.

If $f_{ab}, \overline{U}$ as functions of R vary little over distances of the order of the range of action, then the system of equations for $f_{ab}, \overline{U}$ is simplified. Thus, for example, in the first (dipole) approximation the equations for the functions $f_{ab}, \overline{U}$ have the form

$$\frac{\partial f_{ab}}{\partial t} + \mathbf{V}\frac{\partial f_{ab}}{\partial \mathbf{R}} + \mathbf{v}\frac{\partial f_{ab}}{\partial \mathbf{r}} - \frac{\partial \Phi}{\partial \mathbf{r}}\frac{\partial f_{ab}}{\partial \mathbf{p}} + e_1\left(\mathbf{r}\frac{\partial}{\partial \mathbf{R}}\right)\mathbf{E}\frac{\partial f_{ab}}{\partial} + e_1\mathbf{E}\frac{\partial f_{ab}}{\partial \mathbf{p}} = 0, \tag{12}$$

$$\operatorname{div}\mathbf{E}(\mathbf{R}, t) = -4\pi e_1 n \frac{\partial}{\partial \mathbf{R}} \int \mathbf{r} f_{ab}(\mathbf{R}, \mathbf{r}, \ , \mathbf{p})\, d\mathbf{r}\, d\ \ d\mathbf{p}. \tag{13}$$

In the quantum case, instead of (3) we use the function (cf. (5))

$$N_{ab} = \frac{1}{(2\pi)^6} \int \rho\left(\mathbf{R} + \frac{1}{2}\hbar\vec{\theta}, \mathbf{r} + \frac{1}{2}\hbar\vec{\tau}, \mathbf{R} - \frac{1}{2}\hbar\vec{\theta}, \mathbf{r} - \frac{1}{2}\hbar\vec{\tau}\right) e^{-i\vec{\theta}\ -i\vec{\tau}\mathbf{p}}. \tag{14}$$

Here ρ is the operator density matrix.

If the spectrum corresponding to the relative motion of particles in pairs is discrete, then instead of (14) we use the function

$$N_{ab}(\mathbf{R}, \ , \mathbf{r}, \mathbf{p}) = \sum_{nm} N_{nm}^{(ab)}(\mathbf{R}, \ ) f_{nm}(\mathbf{r}, \mathbf{p}), \tag{15}$$

where

$$N_{nm}(\mathbf{R}, \ , t) = \frac{1}{(2\pi)^3} \int \rho_{nm}\left(\mathbf{R} + \frac{1}{2}\hbar\vec{\theta}, \mathbf{R} - \frac{1}{2}\hbar\vec{\theta}, t\right) e^{-i\vec{\Pi}\vec{\theta}}\, d\vec{\theta},$$

$$f_{nm}(\mathbf{r}, \mathbf{p}) = \frac{1}{(2\pi)^3} \int \Psi_m^*\left(\mathbf{r} - \frac{1}{2}\hbar\vec{\tau}\right) \Psi_n\left(\mathbf{r} + \frac{1}{2}\hbar\vec{\tau}\right) e^{-i\vec{\tau}\mathbf{p}}\, d\vec{\tau},$$

Ψ_n are eigenfunctions of the operator $\hat{H} = \hat{p}^2/2\mu + \Phi(|\mathbf{r}|)$.

The equation for the function $N_{nm}^{(ab)}(\mathbf{R},\ ,t)$ has the form

$$\frac{\partial N_{nm}}{\partial t}+\mathbf{V}\frac{\partial N_{nm}}{\partial \mathbf{R}}=\frac{1}{i\hbar}(E_n-E_m)N_{nm}+$$

$$+\frac{e_1}{i\hbar(2\pi)^3}\int\sum_k\left(U_{nk}^{(-)}\left(\mathbf{R}+\frac{1}{2}\hbar\vec{\theta}\right)N_{km}(\mathbf{R},\ ')-\right.$$

$$\left.-N_{nk}(\mathbf{R},\ ')U_{km}^{(-)}\left(\mathbf{R}-\frac{1}{2}\hbar\vec{\theta}\right)\right)e^{i\vec{\theta}(\ '-\ )}\,d\theta. \tag{16}$$

The equation for U and expression (9) remain the same.

Equation (16) is substantially simplified if the motion is classical with respect to the variables, while with respect to the variables $\mathbf{r},\mathbf{p}$ one uses the dipole (or higher) approximation.

In the approximation of "free" charges, for the first moments $\overline{N}_{ab},\overline{U}$ from (15), (16) there follows a self-consistent system of equations for the quantum distribution functions $f_a,f_b,\overline{U}$ (^{6},^{7}).

In a more general case, from (15), (16) there follows a system of quantum self-consistent equations for pairs of charged particles.

The equations presented here and the corresponding equations for interacting neutral particles are used to obtain kinetic equations taking into account the "internal" degrees of freedom, and also to solve certain problems in the theory of nonlinear polarization.

In particular, with the aid of equation (16) a kinetic equation has been obtained for the quantum distribution function $\overline{N}_{nn}(\ ,t)$. In the equilibrium case $\overline{N}_{nn}(\ ,t)$ is the Maxwell distribution in and the Boltzmann distribution in E_n.

For a system of molecules with two levels an expression has been obtained for the polarization with allowance for saturation and the thermal motion of the molecules. In the approximation in which the relaxation is characterized by two times τ_1,τ_2 and

electric field $\mathbf{E}(\mathbf{R},t)=\mathbf{E}\cos(\omega t-\mathbf{kR})$, the expression for the polarization vector $\mathbf{P}(\mathbf{R},t)$ has the form

$$\mathbf{P}(\mathbf{R},t)=-\frac{e^2n|\mathbf{r}_{12}|^2}{\hbar}\int d\mathbf{P}\,\left(\rho_2^{(0)}(\mathbf{P})-\rho_1^{(0)}(\mathbf{P})\right)\mathbf{E}\times\left[\frac{(\omega_{21}-\omega+\mathbf{kV})\cos(\omega t-\mathbf{kR})+\dfrac{1}{\tau_2}\sin(\omega t-\mathbf{kR})}{(\omega_{21}-\omega+\mathbf{kV})^2+\dfrac{1}{\tau_2^2}+\dfrac{\tau_1}{\tau_2}\dfrac{e^2}{\hbar^2}|\mathbf{r}_{12}|^2E^2}\right]. \tag{17}$$

Here $\rho_2^{(0)}(\mathbf{P})$, $\rho_1^{(0)}(\mathbf{P})$ are the populations for molecules with momentum $\mathbf{P}$. If the thermal motion is not taken into account $\left(\rho_n^{(0)}\mathbf{P} = \rho_n\delta(\mathbf{P})\right)$, then expression (17) coincides with the known expression for the polarization vector with allowance for saturation.

Expression (17) corresponds to that given in the book [8].

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Note: Figure translations are in progress. See original paper for figures.