

Phase density method: A microscopic description of the gas of neutral particles

Valery V. Yevstafiev

Institute of Solar-Terrestrial Physics SD RAS, Irkutsk 664033, Russia

(Received 7 March 2000; revised manuscript received 31 May 2001; published 24 September 2001)

This paper is devoted to the construction of local microscopic equations describing the evolution of the gas that is treated as a system of a finite number N of point particles placed in a given fixed volume of space. It is assumed that, given an arbitrary motion of the particles, the state of each of them is characterized by a set s ($1 \leq s < \infty$) of dynamic nonzero variables. Such a set represents a point in some $3s$ -dimensional phase space. The notion of the s -th order phase density is introduced, and it is shown that the hierarchy of densities satisfies an infinite system of coupled integrodifferential equations. The structure of the equations suggests the conditions, under which they can be transformed to a closed system of p differential equations: a functional relation between the $(p+1)$ th and the other p dynamic variables must be specified. For the gas of neutral particles, such a relation is found from ordinary equations of motion of particles ($p=2$). However, the acceleration of an individual particle turns out to be a function not only of its coordinates and velocity but also of the coordinates and velocity of the other $(N-1)$ particles of the system having the role of the field sources. The presence of an additional coupling leads to the “splitting” of the second of the two remaining evolution equations into a closed system of N equations for so-called multiparticle phase densities. The physical meaning of these equations and their possible implications for the kinetic theory of gases are discussed. It is stressed that a similar system of microscopic equations can be constructed for any microscopic quantities of the system of particles under consideration.

DOI: 10.1103/PhysRevE.64.041201

PACS number(s): 51.10.+y, 45.05.+x, 45.50.-j, 45.90.+t

I. INTRODUCTION

The phase density method was first suggested in a paper of Klimontovich concerned with a local microscopic description of the plasma treated as a system of a large number of N charged point particles that move according to the known law in a given volume of space [1]. The method is a technique for constructing the equation for microscopic phase density, which is a local characteristic of the system. It also worked well for describing systems of such complicated objects as atoms, molecules, and the like, which were regarded as bound states of point particles of a different sort [2]. The importance of such equations lies in the fact that kinetic equations of a general form can be constructed using them [2–7].

It is known that each particle of the system has the role of the object acted upon by the fields of the other $(N-1)$ particles and of external (relative to the system) sources, and the role of the field source for the other particles at a time. To obtain the closed microscopic equation, Klimontovich used the “self-action” approximation implying that a change in particle momentum is possible under the action not only of external (relative to it) fields but also of its own field. Within the context of the microscopic description of a single system of particles, such an approximation is physically meaningless since it introduces divergent terms into the theory [7,8]. Knowing that such systems are nonexistent in nature, Klimontovich stresses that his approximation has a technical character and that, when the occasion requires, the contribution that is determined by self-action, can always be excluded. As an illustration, he even develops a “correct,” now nonclosed equation, but right there everything ends [2].

In spite of the approximate character of the microscopic equation, Klimontovich and other authors managed to obtain,

on its basis, macroscopic results in agreement with universally known ones, and they took it as circumstantial evidence for the validity of the equation itself [2,6–8]. Yet this fact in no way was associated with the approximation itself: an analysis of their calculations shows that the application of the procedure of averaging the microscopic equation over an ensemble, involving the method of moments and various assumptions [2], leads to an implicit compensation of the contribution determined by self-action. Nevertheless, the idea of switching over from microscopic to kinetic equations seems quite attractive. It is necessary merely to derive “correct” microscopic equations and to point out the rule of such a switchover. In this paper, an attempt is made to solve the former of these problems.

This treatment starts from the one-component gas whose particles move in an arbitrary fashion in a given volume of space. Such a motion will be characterized by an infinite number of dynamic variables, which necessitates introducing a notion of the $3s$ -dimensional phase space ($1 \leq s < \infty$), and of s th-order phase density. The use of an extended phase density method, based on such properties of particles as their point character and the constancy of their number in the system, leads to an infinite system of coupled integrodifferential equations for phase densities. Analysis of the structure suggests the condition for “terminating” them and obtaining a closed system of p differential equations: the presence of a coupling between the $(p+1)$ th and the other p dynamic variables. The explicit form of the coupling is determined in each particular problem.

For the neutral gas, such a coupling is defined by the ordinary equation of motion ($p=2$). In this case, the acceleration of an individual particle depends not only on its dynamic variables, as is required by the termination condition, but also on the dynamic variables of the other $(N-1)$ par-

ticles. The presence of an additional coupling leads to the ‘‘splitting’’ of the second of the two remaining evolution equations into a closed system of N equations for so-called multiparticle phase densities. Such a system of $(N+1)$ differential equations describes the microscopic evolution of a single system of N particles rather than of their ensemble.

II. GENERAL SCHEME

Let there be, in a fixed volume of space V^* , a sufficient amount of gas consisting of a constant number N of moving particles of the same sort (results are easily generalized to the case of a multicomponent gas). The sufficiency implies that the linear size of the volume is much larger than the mean distance between particles. The constancy of the number of particles signifies that the gas supports only those physical processes, which as time progresses, (a) do not change the nature of particles, and (b) confine them to a given volume. If, in this case, (c) the mean distance between particles is much larger than their diameter, then such a gas may be represented as a system of point particles. Their motion is described by methods of classical mechanics [9,10].

In the dynamic approach, the state of an arbitrary i th particle at the time t is determined by the values of two dynamic variables: the radius vector $\mathbf{r}_i(t)$ and the velocity $\mathbf{v}_i(t)$, ($i = \bar{1}, \bar{N}$). It is obvious that they are not independent quantities [2]. By specifying the state of all particles at the initial time t_0 and integrating N equations of motion, it is possible, in principle, to calculate the radius vectors of particles for every subsequent instant of time. The solution of this problem will also make it possible to consider the evolution of such physical quantities as the momentum of the system, its kinetic energy, etc., which represent the specified functions of dynamic variables of N particles.

The local approach treats the properties not of the entire system of particles but only of those that at the time t ($t > t_0$) are in the volume V ($V \in V^*$). The corresponding (local) physical quantity then represents a limited (by the volume V) integral over the coordinate space \mathbf{r} of the local microscopic function. Functions of this kind are determined by the condition that in the limit $V \rightarrow V^*$ the local physical quantity coincides with the quantity obtained in the dynamic approach. For local functions, a method of constructing differential equations, the phase density method, is known [2]. The evolution of local physical quantities is studied either on the basis of their determination (by substituting into it the solution of the microscopic equation) or through a direct construction and solution of differential equations for these quantities themselves.

The simplest local function is represented by the microscopic particles number density, $n(\mathbf{r}, t)$, specified in a continuous space of coordinates by the condition

$$\int_{V^*} n(\mathbf{r}, t) d\mathbf{r} = N, \quad (1)$$

i.e., the integral of $n(\mathbf{r}, t)$ over the entire volume of the system is equal to a total number of particles in it, here $d\mathbf{r} = dr_x dr_y dr_z$. The number of particles in the volume V at the

time t is also equal to the integral of $n(\mathbf{r}, t)$ taken over this volume, however. It is obvious that, because of the continuous motion of the particles, the number of particles in this volume will be different at different instants of time.

To obtain the equation for $n(\mathbf{r}, t)$, the density is represented as the sum of the following Dirac δ functions over N particles of the system:

$$n(\mathbf{r}, t) \equiv \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i(t)), \quad (2)$$

where $\delta(\mathbf{r} - \mathbf{r}_i(t)) = \delta(r_x - r_{xi}(t))\delta(r_y - r_{yi}(t))\delta(r_z - r_{zi}(t))$. Such a representation satisfies the condition (1); it should be noted, however, that its some terms there can be infinite. This means that in the representation (2) the quantity $n(\mathbf{r}, t)$ is not a physical quantity: it belongs to the class of so-called generalized functions. Such functions reflect some preassigned properties of the representing quantity and are introduced with the purpose of constructing the respective differential equations, following the known recipes. In the present case this implies differentiating the expression (2) with respect to the time t as a composite (time-dependent in terms of dynamic variables) function, in view of the properties of the δ function and the condition $N = \text{const}$. The terms of the resulting intermediate equation are then expressed either in terms of the quantity $n(\mathbf{r}, t)$ itself or in terms of some other generalized function.

Note that to construct the equation, Klimontovich used the microscopic phase density $\mathcal{N}(\mathbf{r}, \mathbf{v}, t)$ specified in a continuous space of coordinates and velocities, \mathbf{r} and \mathbf{v} (which he called the six-dimensional phase space) by the expression,

$$\mathcal{N}(\mathbf{r}, \mathbf{v}, t) \equiv \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i(t))\delta(\mathbf{v} - \mathbf{v}_i(t)). \quad (3)$$

This choice is associated with the assumption that it is possible to express in terms of the quantity $\mathcal{N}(\mathbf{r}, \mathbf{v}, t)$ the microscopic densities of almost all known physical quantities. In order for the resultant internal force to be included in their number, the self-action approximation was used, the meaning of which has already been discussed above. Eventually the resulting differential equation for $\mathcal{N}(\mathbf{r}, \mathbf{v}, t)$ becomes closed. This study will show that there is no need for such an approximation and that a consistent application of the phase density method permits us to construct microscopic equations. Furthermore, there naturally arise the notions of microscopic densities of different physical quantities, and differential equations corresponding to them.

A. The coupling equation for phase densities

It will be assumed that the motion of particles in the system under consideration proceeds in an arbitrary fashion, i.e., the laws of their motion are not predetermined. This means that for any i th particle ($i = \bar{1}, \bar{N}$) the time derivatives of its radius vector from the first to infinite orders will be nonzero time functions. We write them as the following s vector quantities (s being an integer, and $1 \leq s < \infty$):

$$\begin{aligned} \mathbf{q}_{1i}(t) = \mathbf{r}_i(t), \quad \mathbf{q}_{2i}(t) = \mathbf{v}_i(t) &\equiv \frac{d\mathbf{r}_i(t)}{dt}, \dots, \mathbf{q}_{si}(t) \\ &= \frac{d^{s-1}\mathbf{r}_i(t)}{dt^{s-1}}, \end{aligned} \quad (4)$$

and we call them the dynamic variables of the i th particle [2]. It is obvious that they are not independent quantities. The first subscript number means the variable number, and the second number corresponds to the particle number. It would appear reasonable that the state of an individual particle must now be characterized not by two dynamic variables but by the entire set of s dynamic variables,

$$Q_{si}(t) = [\mathbf{q}_{1i}(t), \mathbf{q}_{2i}(t), \dots, \mathbf{q}_{si}(t)]. \quad (5)$$

It will be shown later in the text that, depending on the law of motion selected, the number s can assume different finite values.

Let us imagine mentally some $3s$ -dimensional continuous space in which at the time t one particular point that is different from the other points, will correspond to each of the N sets of the dynamic variables of Eq. (5). Call this space the phase space, and let the following s vectors be used as its independent variables

$$\mathbf{q}_1 = \mathbf{r}, \quad \mathbf{q}_2 = \mathbf{v}, \quad \mathbf{q}_3, \quad \dots, \quad \mathbf{q}_s, \quad (6)$$

where the subscript number means the phase variable number. It is obvious that the phase and dynamic variables with the same number have the same physical dimensions. In this connection, the first two vectors in Eq. (6) are shown coincident with the variables of an ordinary six-dimensional phase space [1]. With the exception of the variable \mathbf{r} , the phase variables of Eq. (6) vary from $-\infty$ to $+\infty$. (In the relativistic case this exception refers also to the variable \mathbf{v} ; its values vary from $-c$ to $+c$, where c is the velocity of light). Let us designate an arbitrary point of the $3s$ -dimensional phase space by the set

$$Q_s = (\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_s), \quad (7)$$

where the subscript number of Q indicates the number of phase variables. By analogy with Eqs. (2) and (3), we determine in the $3s$ -dimensional phase space the s -order phase density

$$n_s = n_s(Q_s, t) = \sum_{i=1}^N \delta(Q_s - Q_{si}(t)), \quad (8)$$

where $\delta(Q_s - Q_{si}(t)) = \prod_{l=1}^s \delta(\mathbf{q}_l - \mathbf{q}_{li}(t))$. Then the quantities $n(\mathbf{r}, t)$ and $\mathcal{N}(\mathbf{r}, \mathbf{v}, t)$ are said to be the phase densities of the first and second orders. All phase densities are local functions since they satisfy the condition

$$\int n_s dQ_s \equiv \int_{V^*} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} n_s d\mathbf{q}_1 \dots d\mathbf{q}_s = N. \quad (9)$$

Next we write the following useful coupling between phase densities of different orders (r being an integer, and $1 \leq r < s$):

$$n_r = \int n_s d\mathbf{q}_{r+1} \dots d\mathbf{q}_s. \quad (10)$$

We start the construction of the equations for phase densities from the quantity n_1 . By taking a time derivative with respect to its both parts and using the known property of differentiation of the δ function, we obtain the following intermediate equation:

$$\frac{\partial n_1}{\partial t} = - \frac{\partial}{\partial \mathbf{q}_1} \sum_{i=1}^N \mathbf{q}_{2i}(t) \delta(\mathbf{q}_1 - \mathbf{q}_{1i}(t)). \quad (11a)$$

The presence of the vector $\mathbf{q}_{2i}(t)$ under the summation sign does not permit the right-hand side (RHS) of Eq. (11a) to be expressed in terms of the quantity n_1 itself. However, if the definition (8) at $s=2$ and the other property of the δ function

$$\mathbf{q}_{2i}(t) = \int_{-\infty}^{\infty} \mathbf{q}_2 \delta(\mathbf{q}_2 - \mathbf{q}_{2i}(t)) d\mathbf{q}_2,$$

are taken into account, then equations (11a) may be written as

$$\frac{\partial n_1}{\partial t} = - \frac{\partial}{\partial \mathbf{q}_1} \int_{-\infty}^{\infty} \mathbf{q}_2 n_2 d\mathbf{q}_2. \quad (11b)$$

This integrodifferential equation is nonclosed: its RHS involves the density n_2 , for its determination it is necessary to construct a new equation. It is obvious that this and all other subsequent equations are nonclosed. A general equation for the s -order phase density will have the form

$$\left(\frac{\partial}{\partial t} + \sum_{l=2}^s \mathbf{q}_l \frac{\partial}{\partial \mathbf{q}_{l-1}} \right) n_s = - \frac{\partial}{\partial \mathbf{q}_s} \sum_{i=1}^N \mathbf{q}_{(s+1)i}(t) \delta(Q_s - Q_{si}(t)) \quad (12a)$$

$$= - \frac{\partial}{\partial \mathbf{q}_s} \int_{-\infty}^{\infty} \mathbf{q}_{s+1} n_{s+1} d\mathbf{q}_{s+1}, \quad (12b)$$

where $2 \leq s < \infty$ [when $s=1$ we have Eqs. (11)].

Equations (11b) and (12b) have an important property: all their terms represent different combinations of phase variables and phase densities only. The system with an infinite number of ‘‘coupled’’ integrodifferential equation (12b) does not permit us to use them in solving applied problems. It is necessary to point out a method enabling us to ‘‘terminate’’ the sequence of these equations. To do so, first we note the existing obvious connection between the number of Eq. (12b) and the number of dynamic variables. Note also that in real media the motion of particles is not an arbitrary one: it is always limited to some extent. Consequently, by establishing the character of limitations for a particular system of particles, it is possible to find the method of termination of Eq. (12b) and to obtain a closed system of equations.

An important role will be played by the $(s+1)$ th dynamic variable of an arbitrary i th particle involved in the RHS of Eq. (12a).

Assume that the particles in the system are moving in such a manner that their dynamic variables with numbers higher than the p th are always zero, i.e., $\mathbf{q}_{(p+1)i} = 0$ ($i = \bar{1}, \bar{N}$). Upon substituting this into the RHS of Eq. (12a), we obtain a closed system of p equations. The last of them turns out to have its RHS equal to zero. It is known that under certain conditions and at the specified initial value of the p -order phase density, this equation can, in principle, be solved. The resulting expression for n_p can be used, with the help of the relation (10), to determine smaller-order phase densities. However, there are situations where it is still necessary to successively solve all the remaining $(p-1)$ equations. To do this, the resulting value of n_p is substituted into the RHS of the preceding $(p-1)$ th equation, and this is solved for n_{p-1} . Its solution, in turn, gives n_{p-1} , which is substituted into the $(p-2)$ th equation, and so forth. It should be noted, however, that the case of the motion of particles under consideration exists almost nowhere; therefore, we turn our attention to a more general method of obtaining a closed system of equations.

B. The evolution equation for phase densities

Assume that the motion of particles in the system obeys such a physical law that may be written as the following relation between the dynamic variables of an arbitrary i th particle:

$$\mathbf{q}_{(p+1)i}(t) = \mathbf{f}(Q_{pi}, t), \quad i = \bar{1}, \bar{N}. \quad (13)$$

Noteworthy here is an explicit time dependence of the RHS. Upon substituting Eq. (13) into Eq. (12a) and taking advantage of the property

$$\mathbf{f}(Q_{pi}, t) \delta(Q_p - Q_{pi}(t)) = \mathbf{f}(Q_p, t) \delta(Q_p - Q_{pi}(t))$$

(it is verified by a direct integration over the phase volume of the system), we arrive at the following closed differential equation:

$$\left(\frac{\partial}{\partial t} + \sum_{l=2}^p \mathbf{q}_l \frac{\partial}{\partial \mathbf{q}_{l-1}} \right) n_p = - \frac{\partial}{\partial \mathbf{q}_p} (\mathbf{f}(Q_p, t) n_p). \quad (14)$$

Since the coefficients of the equation represent the known functions of phase variables, this equation can, in principle, be solved. Smaller-order phase densities are then obtained using the relation (10).

This does not complete the microscopic local description of the system of particles: it is still necessary to consider the above-mentioned problem of introducing into the theory other local functions and of constructing the evolution equations for them. One way to solve this problem is as follows. Since Eqs. (12b) involve integrals of the same type, they may be represented as the following functions:

$$\int_{-\infty}^{\infty} \mathbf{q}_k n_k d\mathbf{q}_k = \mathbf{U}_k(Q_{k-1}, t), \quad (15)$$

where $2 \leq k \leq p$. It is obvious that the vector \mathbf{U}_k is a local function and represents the density of quantity \mathbf{q}_k in the $3(k-1)$ -dimensional phase space. Let the symbol $a = 1, 2, 3$, involved on the lower right of the vector, designate its Cartesian components. Then, by multiplying each k th of the $(p-2)$ Eq. (12b), as well as Eq. (14) by the quantity $(q_k)_a$ and integrating over \mathbf{q}_k , we obtain the following system of p microscopic equations:

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + \sum_{l=2}^{p-1} \mathbf{q}_l \frac{\partial}{\partial \mathbf{q}_{l-1}} \right) (U_p)_a + \frac{\partial}{\partial \mathbf{q}_{p-1}} \int_{-\infty}^{\infty} \mathbf{q}_p (q_p)_a n_p d\mathbf{q}_p \\ & = \int_{-\infty}^{\infty} [f(Q_p, t)]_a n_p d\mathbf{q}_p, \end{aligned} \quad (16a)$$

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + \sum_{l=2}^{k-1} \mathbf{q}_l \frac{\partial}{\partial \mathbf{q}_{l-1}} \right) (U_k)_a + \frac{\partial}{\partial \mathbf{q}_{k-1}} \int_{-\infty}^{\infty} \mathbf{q}_k (q_k)_a n_k d\mathbf{q}_k \\ & = \int_{-\infty}^{\infty} (U_{k+1})_a d\mathbf{q}_k, \end{aligned} \quad (16b)$$

$$\frac{\partial n_1}{\partial t} = \frac{\partial \mathbf{U}_2}{\partial \mathbf{q}_1}. \quad (16c)$$

When deriving Eq. (16), we used the following important property of the integrals:

$$\int_{-\infty}^{\infty} \frac{\partial}{\partial \mathbf{q}_k} [\Psi(Q_k, t) n_k] d\mathbf{q}_k = 0, \quad (17)$$

where the vector $\Psi(Q_k, t)$ is an arbitrary function of phase variables. Note that the system (16) involves terms that do not contain the quantity \mathbf{U}_k . They arise due to the fact that the relation (15) does not permit the densities n_k to be uniquely expressed in terms of \mathbf{U}_k . For this reason, when it is necessary to find the expressions for \mathbf{U}_k , it is more convenient to solve first the system of equations for phase densities and then to use Eq. (15).

There exists an alternative method of overcoming the above-mentioned problem of introducing new local functions. Using Eq. (8), we represent the quantity \mathbf{U}_k as

$$\mathbf{U}_k = \sum_{i=1}^N \mathbf{q}_{ki} \delta(Q_{k-1} - Q_{(k-1)i}(t)) \quad (18a)$$

$$= \mathbf{u}_k(Q_{k-1}, t) n_{k-1}, \quad (18b)$$

where $2 \leq k \leq p$. We can verify that by applying the phase density method to Eq. (18a), we obtain exactly the system of equations (16). It is easy to see that by using this method it is possible to construct microscopic equations for any local function composed of phase variables and of the phase densities. By representing the integral of Eq. (15) as Eq. (18b), it is possible to introduce into consideration a further new quantity $\mathbf{u}_k(Q_{k-1}, t)$, having the meaning of the mean value

of the variable \mathbf{q}_k in the $3(k-1)$ -dimensional phase space. Let us call it the microscopic value of the quantity \mathbf{q}_k . In the particular case where $k=2$, substitution of Eq. (18b) into Eq. (16c) gives the equation coinciding in its form with the macroscopic continuity equation. The quantity $\mathbf{u}_2(Q_1, t)$ will have the role of the microscopic value of the velocity \mathbf{q}_2 in this equation.

III. THE GAS OF NEUTRAL PARTICLES

In real gases the motion of particles is almost always non-relativistic and therefore obeys a classical law of motion [2,9,10]. For an arbitrary i th particle ($i=\bar{1}, \bar{N}$) of the one-component gas, it is written as

$$m_i \mathbf{q}_{3i}(t) = \mathbf{F}_i(t), \quad (19)$$

where $\mathbf{q}_{3i}(t)$ is acceleration, and $m_i = m$ is the mass of the i th particle. The vector $\mathbf{F}_i(t)$ represents the force arising when the i th particle (at the time t) is acted upon by the total field produced both by $(N-1)$ particles surrounding this particle and by external (relative to the system) sources. Recall that the motion of the particles will be nonrelativistic and the particles themselves will remain point objects when the magnitude of each field acting on them is sufficiently small. The superposition principle holds for such fields: the action of the total field causes the same change in particle momentum as does the vector sum of all individual fields. The same holds also true for the forces

$$\mathbf{F}_i(t) = \mathbf{F}_{0i}(t) + \sum_{\substack{j=1 \\ (j \neq i)}}^N \mathbf{F}_{ij}(t). \quad (20)$$

Here $\mathbf{F}_{0i}(t)$ and $\mathbf{F}_{ij}(t)$ represent the actions of the resultant field of external sources, and of the field produced by the j th particle, respectively. The condition $i \neq j$ implies that the i th particle of the system cannot be a source of the field for itself. In emphasizing this role, we shall call the particle whose parameters are related by Eq. (19), the peculiar particle; with respect to it, all the other $(N-1)$ particles represent sources of internal fields. It should be noted that the selection of the law of motion (13) in the form (19) specifies the phase space of the system of particles to be six-dimensional. This permits us to return to the symbols that have already been partly used in Sec. II: the vectors \mathbf{q}_1 and \mathbf{q}_2 are replaced by \mathbf{r} and \mathbf{v} and the quantities n_1, n_2 [see Eq. (8)] are substituted for by $n(\mathbf{r}, t), \mathcal{N}_1(x, t) = \mathcal{N}(\mathbf{r}, \mathbf{v}, t)$ where $x = (\mathbf{r}, \mathbf{v})$.

In particular problems, the sources of external fields are considered given. This implies that the external resultant force may be represented as a radius-vector function of the peculiar particle and of time t (if external sources produce time-dependent fields), $\mathbf{F}_{0i}(t) = \mathbf{F}_0(\mathbf{r}_i(t), t)$. The internal force $\mathbf{F}_{ij}(t)$ for the neutral gas is expressed in terms of the ‘‘potential energy of interaction’’ $\Phi_{ij}(t)$. In the subsequent discussion, in the expressions for fields and forces the verti-

cal bar will separate the parameters of the peculiar particle and of the source particles. Then $\Phi_{ij}(t) = \Phi(|\mathbf{r}_i(t) - \mathbf{r}_j(t)|) = \Phi(\mathbf{r}_i(t)|\mathbf{r}_j(t))$, and

$$\mathbf{F}_{ij}(t) = - \frac{\partial \Phi_{ij}(t)}{\partial \mathbf{r}_i(t)} = \mathbf{F}(\mathbf{r}_i(t)|\mathbf{r}_j(t)), \quad (i \neq j). \quad (21)$$

Hence it follows that the time dependence of the internal forces has an implicit character, and the parameters of the source and of the peculiar particle are taken at the same time t . However, with the finite propagation velocity of the fields, the time of emission of the field by the j th particle, t'_j must differ from t by the delay time $t - t'_j > 0$. The use of $t = t'_j$ in the expression (21) is motivated by the short-lived character of the field $\Phi_{ij}(t)$ when at every instant of time the peculiar particle is acted upon by fields only of several most closely lying source particles. Furthermore, the delay time will be negligibly small compared with the characteristic time of the macroscopic processes occurring in the system. It should be noted that the delay times can differ from each other by several times, and this difference does not depend on the velocity of the particles. It is particularly important to take this difference into account in the microscopic description of the gas of charged particles acting on one another through far-ranging electromagnetic fields. The delay times for them can also differ considerably.

Thus the acceleration of the peculiar particle depends not only on its dynamic variables, as is required by the condition (13), but also on the variables of the other particles of the system. The presence of an additional coupling does not permit the results from the preceding section to be used directly; therefore, it is necessary again to invoke the system of equations (12b). Using Eq. (19), we transform it into a system of two equations

$$\frac{\partial n(\mathbf{r}, t)}{\partial t} = - \frac{\partial}{\partial \mathbf{r}} \int_{-\infty}^{\infty} \mathbf{v} \mathcal{N}_1(x, t) d\mathbf{v}, \quad (22a)$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \frac{\partial}{\partial \mathbf{r}} \right) \mathcal{N}_1(x, t) = - \frac{\partial}{\partial \mathbf{v}} \sum_{i=1}^N \mathbf{q}_{3i}(t) \delta(x - x_i(t)). \quad (22b)$$

We now write Eq. (22b) in the variables of the phase space; to do this, we represent the force of Eq. (21) as an integral over the entire volume of the phase space occupied by the system:

$$\mathbf{F}_{ij}(t) = \int_{V^*} \int_{-\infty}^{\infty} \mathbf{F}(\mathbf{r}_i(t)|\mathbf{r}') \delta(x' - x_j(t)) dx', \quad (23)$$

where $dx' = d\mathbf{r}' d\mathbf{v}'$. On substituting into Eq. (22b) the expression (19), in view of Eqs. (20), (21), and (23), we arrive at the following evolution equation for the density $\mathcal{N}_1(x, t)$:

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + \mathbf{v} \frac{\partial}{\partial \mathbf{r}} + \mathbf{F}_0(\mathbf{r}, t) \frac{\partial}{\partial \mathbf{p}} \right) \mathcal{N}_1(x, t) \\ & = - \int \mathbf{F}(\mathbf{r}|\mathbf{r}') \frac{\partial \mathcal{N}_1(x, t) \mathcal{N}_1^{(x)}(x', t)}{\partial \mathbf{p}} dx'. \quad (24) \end{aligned}$$

The integral here is written in the sense of Eq. (23), $\mathbf{p}=m\mathbf{v}$, and $\mathbf{F}(\mathbf{r}|\mathbf{r}')$ stands for the force, with which the field from the source particle will be acting on some peculiar particle, provided that both of them will be at the points \mathbf{r} and \mathbf{r}' .

At this point it is necessary to explain that the point x , like any other point of the phase space, is chosen arbitrarily; therefore, at the time t this point may not contain a particle. Nevertheless, Eq. (24) remains valid, although it turns into a usual zero identity. Consequently, the nontrivial meaning is acquired by Eq. (24) only at the point of the phase space, at which at the time t one of N particles will reside. Such a point will be said to be the peculiar point of the phase space and, in this sense, we make the convention that there is an action of the fields on the peculiar point.

Note that under the integral in Eq. (24) we have, together with $\mathcal{N}_1(x,t)$, a new quantity

$$\mathcal{N}_1^{(x)}(x',t) = \mathcal{N}_1(x',t) - \delta(x-x'), \quad (25)$$

which differs from $\mathcal{N}_1(x',t)$ in that the peculiar point x is excluded from it. This imparts to the quantity of Eq. (25) the meaning of the phase density of the number of sources (for the point x) at the point x' . It is obvious that it is a local function: the integral

$$\int \mathcal{N}_1^{(x)}(x',t) dx' = N-1, \quad (26)$$

is equal to the number of sources for the peculiar point x . The fact that the quantity $\mathcal{N}_1^{(x)}(x',t)$ involved in Eq. (24) makes it nonclosed; however, the evolution equation required for finding this quantity is more conveniently constructed for the product

$$\begin{aligned} \mathcal{N}_1(x,t)\mathcal{N}_1^{(x)}(x',t) &\equiv \mathcal{N}_2(x,x',t) \\ &= \sum_{\substack{i,j=1 \\ (j \neq i)}}^N \delta(x-x_i(t))\delta(x'-x_j(t)). \end{aligned} \quad (27)$$

If only the RHS of Eq. (27) is taken into account, then the quantity $\mathcal{N}_2(x,x',t)$ represents a function that is symmetric with regard to the permutation of the variables x and x' . For this reason, it was labeled as the two-particle phase density, and the quantity $\mathcal{N}_1(x,t)$ received the name one-particle phase density [2].

On the other hand, since in Eq. (24) x is a peculiar point and the point x' belongs in the phase space of sources, these points have a different physical meaning. This difference becomes obvious if we take into account the nonzero, even if negligibly small, delay time. In this case the points x and x' become ‘‘tied’’ to the times t and t' , with $t > t'$. In the subsequent discussion the delay will be neglected; however, when carrying out a physical interpretation of results obtained, it should not be omitted. We believe that this remark is of particular importance in the context of the well-known problem of the time irreversibility of kinetic and hydrodynamic equations [2,11]. Nevertheless, in obtaining the evolution equations for the quantity $\mathcal{N}_2(x,x',t)$, the points x and

x' are formally considered to be two different and independent peculiar points. [When the occasion requires, the difference of the times t and t' may be taken into account in Eq. (24) in the process of integration.] Hence,

$$\begin{aligned} &\left(\frac{\partial}{\partial t} + \mathbf{v} \frac{\partial}{\partial \mathbf{r}} + \mathbf{v}' \frac{\partial}{\partial \mathbf{r}'} + \mathbf{F}_0(\mathbf{r},t) \frac{\partial}{\partial \mathbf{p}} + \mathbf{F}_0(\mathbf{r}',t) \frac{\partial}{\partial \mathbf{p}'} \right) \mathcal{N}_2(x,x',t) \\ &= - \int \mathbf{F}(\mathbf{r}|\mathbf{r}'') \frac{\partial}{\partial \mathbf{p}} [\mathcal{N}^{(x)}(x'',t) \mathcal{N}_2(x,x',t)] dx'' \\ &\quad - \int \mathbf{F}(\mathbf{r}'|\mathbf{r}'') \frac{\partial}{\partial \mathbf{p}'} [\mathcal{N}^{(x')}(x'',t) \mathcal{N}_2(x,x',t)] dx''. \end{aligned} \quad (28)$$

Noteworthy are the similarity of the operators involved in the left-hand side (LHS) of Eqs. (24) and (28), and the correspondence of their number to the number of peculiar points. The integrals in Eq. (28) describe the contribution to the evolution made by the quantity $\mathcal{N}_2(x,x',t)$ made by the mutual action of the peculiar points x and x' , as well as of the action of particles from the phase space of sources on them.

We now express the bracketed products of phase densities in terms of a three-particle phase density [cf. Eq. (27)]

$$\begin{aligned} \mathcal{N}_3(x,x',x'',t) &= \sum_{\substack{i,j,k=1 \\ (j \neq i \neq k)}}^N \delta(x-x_i(t))\delta(x'-x_j(t)) \\ &\quad \times \delta(x''-x_k(t)). \end{aligned} \quad (29)$$

With a rather unwieldy manipulation we get

$$\begin{aligned} \mathcal{N}^{(x)}(x'',t)\mathcal{N}_2(x,x',t) &= \mathcal{N}_3(x,x',x'',t) \\ &\quad + \delta(x''-x')\mathcal{N}_2(x,x',t), \\ \mathcal{N}^{(x')}(x'',t)\mathcal{N}_2(x,x',t) &= \mathcal{N}_3(x,x',x'',t) \\ &\quad + \delta(x''-x)\mathcal{N}_2(x,x',t). \end{aligned}$$

In view of these expressions, Eq. (28) takes the form

$$\begin{aligned} &\left(\frac{\partial}{\partial t} + \mathbf{v} \frac{\partial}{\partial \mathbf{r}} + \mathbf{v}' \frac{\partial}{\partial \mathbf{r}'} + [\mathbf{F}_0(\mathbf{r},t) + \mathbf{F}(\mathbf{r}|\mathbf{r}')] \frac{\partial}{\partial \mathbf{p}} \right. \\ &\quad \left. + [\mathbf{F}_0(\mathbf{r}',t) + \mathbf{F}(\mathbf{r}'|\mathbf{r}')] \frac{\partial}{\partial \mathbf{p}'} \right) \mathcal{N}_2(x,x',t) \\ &= - \int \left[\mathbf{F}(\mathbf{r}|\mathbf{r}'') \frac{\partial}{\partial \mathbf{p}} + \mathbf{F}(\mathbf{r}'|\mathbf{r}'') \frac{\partial}{\partial \mathbf{p}'} \right] \mathcal{N}_3(x,x',x'',t) dx''. \end{aligned} \quad (30)$$

The LHS now involves two terms that take explicitly into account the contribution of the mutual action of the peculiar points x and x' to the evolution of the quantity $\mathcal{N}_2(x,x',t)$. The RHS retains only those terms that describe the contribution from the action (on these points) of the fields from the remaining $(N-2)$ particles of the system. Equation (30), like Eq. (24), is also nonclosed, but now because of the in-

volvement of the quantity $\mathcal{N}_3(x, x', x'', t)$. It is obvious that the evolution equation for this quantity will contain a four-particle density, etc. As a result, we get a system of coupled equations for multiparticle phase densities.

The need to distinguish, in the subsequent treatment, a large number of points of the six-dimensional phase space induces us to introduce the following designations of the phase variables:

$$x = x^{(1)}, \quad x' = x^{(2)}, \quad x'' = x^{(3)}, \dots \quad (31)$$

It can be directly verified that the properties of an n -particle phase density (as a local function) will be defined by the relation

$$\int \mathcal{N}_n(x^{(1)}, \dots, x^{(n)}, t) dx^{(1)} \dots dx^{(n)} = \frac{N!}{(N-n)!}. \quad (32)$$

Hence, when $1 \leq n < N$ (n being an integer), the evolution equation has the form

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + \sum_{l=1}^n \left[\mathbf{v}^{(l)} \frac{\partial}{\partial \mathbf{r}^{(l)}} + m \mathbf{w}_n(\mathbf{r}^{(l)}, t) \frac{\partial}{\partial \mathbf{p}^{(l)}} \right] \right) \\ & \times \mathcal{N}_n(x^{(1)}, \dots, x^{(n)}, t) \\ & = - \int \sum_{l=1}^n \mathbf{F}(\mathbf{r}^{(l)} | \mathbf{r}^{(n+1)}) \frac{\partial}{\partial \mathbf{p}^{(l)}} \\ & \times \mathcal{N}_{n+1}(x^{(1)}, \dots, x^{(n+1)}, t) dx^{(n+1)}, \quad (33) \end{aligned}$$

where, for sake of evidence, the following notation is introduced:

$$m \mathbf{w}_n(\mathbf{r}^{(l)}, t) = \mathbf{F}_0(\mathbf{r}^{(l)}, t) + \sum_{\substack{k=1 \\ (k \neq l)}}^n \mathbf{F}(\mathbf{r}^{(l)} | \mathbf{r}^{(k)}), \quad l = \bar{1}, \bar{N}. \quad (34)$$

Equation (33) will have a nontrivial meaning if n equals the number of peculiar points. The expression (34) represents the portion of the force, with which an arbitrary peculiar point $x^{(l)}$ at the time t is acted upon by external fields and by fields produced by the other $(n-1)$ peculiar points. Consequently, the LHS of Eq. (33) involves n terms that take into account the contribution to the evolution from the n -particle density of the external fields, and $n(n-1)$ terms that take into account the mutual action of the peculiar points. Under the integral sign on the RHS of Eq. (33) there remain n terms that take into account the action on each of the n peculiar points $(N-n)$ exerted by the particles from the phase space of sources. Note that any n out of N particles can reside at these points, and in any order. The relation (32) does determine the number of possible ways of their arrangement.

Since none of the particles of the system can be at two different points of the space at a time, the number of peculiar points cannot exceed a total number of particles in the system, N . Thus all densities with $n > N$ will be zero, and the equation for N -particle density will represent Eq. (33) with its RHS equal to zero;

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + \sum_{l=1}^N \left[\mathbf{v}^{(l)} \frac{\partial}{\partial \mathbf{r}^{(l)}} + m \mathbf{w}_N(\mathbf{r}^{(l)}, t) \frac{\partial}{\partial \mathbf{p}^{(l)}} \right] \right) \\ & \times \mathcal{N}_N(x^{(1)}, \dots, x^{(N)}, t) = 0. \quad (35) \end{aligned}$$

This means that when $n = N$, all conceivable particles of the system will be distributed in the peculiar points, and hence none of the particles will be left in the phase space of sources. The quantity $m \mathbf{w}_N(\mathbf{r}^{(l)}, t)$ now is a total force, with which an arbitrary peculiar point $x^{(l)}$ is acted upon by external fields, and by fields produced by all the other $(N-1)$ peculiar points.

Thus, microscopic evolution equations for multiparticle densities is equal to $(N+1)$: in addition to the newly obtained Eqs. (33), (34), and (35) it is necessary to include Eq. (22a), which is left after the termination of the system (12b). Equation (35) now has a closed form. Under certain conditions, it can be solved, and the determined values of the N -particle density can then be used to find the other densities by taking advantage, for this purpose, of the following relation:

$$\begin{aligned} & \mathcal{N}_n(x^{(1)}, \dots, x^{(n)}, t) \\ & = \frac{1}{(N-n)!} \int \mathcal{N}_N(x^{(1)}, \dots, x^{(N)}, t) dx^{(n+1)} \dots dx^{(N)}, \quad (36) \end{aligned}$$

where $1 \leq n < N$. The relation (36) is readily verified by direct integration. It should be noted that to solve equation (35) requires a knowledge of the initial value of the N -particle density that, in turn, requires specifying $6N$ initial values of dynamic variables. In real gases, this number is too large; therefore, the solution of Eq. (35) is impracticable. In this sense, the microscopic description of a system of particles using the phase density method does not offer any advantages over the dynamic approach [2]. The attractiveness of Eqs. (33) and (35) lies in their structure and in the fact that they are written in terms of continuous phase variables. Recall that the method was developed [1,2,4] for constructing such a microscopic equation that could be used directly in the procedure of proceeding to an approximate (incomplete) macroscopic description of the system of particles.

However, the extension of the phase density method and its successive application in this study enabled us to obtain a whole system of $(N+1)$ microscopic equations rather than one equation. Furthermore, their form resembles the widely known equations of Born-Bogoliubov-Green-Kirkwood-Yvon (BBGKY), describing the evolution of an ensemble of systems [2]. Yet our equations differ fundamentally from BBGKY equations in that they describe the microscopic evolution of a single particular system of N particles. Besides, microscopic multiparticle phase densities are determinate quantities, while the generally accepted distribution functions of the probability density are not. Another important property of such microscopic equations is emphasized by the following citation from Koga [8]: ‘‘Any experiment is conducted within a finite time interval with a single system of

particles that is not in a state of thermal equilibrium. Therefore, results of measurements are influenced by the evolution of just this particular system, instead of an ensemble of such systems.' Nevertheless, the presence of the above-mentioned similarity is indicative of a profound connection between the two different levels of description of a system of particles.

In spite of some difficulties, this connection can be realized by analogy with a traditional method used by Klimontovich, namely, by averaging the microscopic equation over an ensemble of systems of particles. However, an alternative procedure is possible, based on the advantages of the local approach used in this study. It implies that any local physical quantity, characterizing the properties of particles in some volume of space V , is expressed in terms of an integral over the space of coordinates, of a particular local function. Using this determination and a system of microscopic equations, it is possible to construct evolution equations for local physical quantities. It should be noted that the merits of both of these methods of proceeding from the microscopic to macroscopic description will be determined by the fact that the various approximate approaches for solving kinetic equations obtained can be justified in terms of the microscopic description. We intend to examine all these issues in one of our subsequent papers.

IV. CONCLUDING REMARKS

The main results, and the conditions under which they have been obtained, may be summarized as follows.

(1) It was assumed that the one-component gas of neutral particles supports only those physical processes that: confine the particles to a certain specified volume of space without

altering the nature of the particles, and conserve their number N unchanged. The microscopic description of such a system of particles was based on the usual local approach of classical mechanics of many bodies.

(2) For an arbitrary motion of particles, characterized by s dynamic variables ($1 \leq s < \infty$), it was necessary to introduce an extended notion of the $3s$ -dimensional phase space and the s -order microscopic phase density specified on it. It was shown that these particles number phase densities satisfy an infinite sequence of coupled integrodifferential equations.

(3) For such systems of particles, in which there exists a connection between the $(p+1)$ dynamic variable of the particle and its other p variables ($1 \leq p < s$), this infinite sequence of equations is transformed into a closed system of p differential equations. The same method was applied to obtain the equations for microscopic densities of other physical quantities.

(4) For a real gas of neutral particles, such a connection exists, and not only does it correspond to the case $p=2$, but it contains an additional dependence on the dynamic variables of the other particles. Taking this factor into account leads us to obtain a system of $(N+1)$ differential equations for so-called multiparticle densities that are now specified on a six-dimensional phase space.

ACKNOWLEDGMENTS

I would like to thank staff members of ISTP Division 1.00, and in particular Dr. I. I. Orlov, Dr. N. V. Ilyin, and Dr. S. I. Mikhailov, for their patience and encouraging discussions. The research reported here would never have been initiated without the financial support of the Russian Foundation for Basic Research, RFBR (93-22-15286).

-
- [1] Yu. L. Klimontovich, *The Statistical Theory of Non-equilibrium Processes in a Plasma* (Pergamon Press, Oxford, 1967).
- [2] Yu. L. Klimontovich, *Statistical Physics* (Harwood Academic Publishers, New York, 1986).
- [3] Yu. L. Klimontovich, *The Kinetic Theory of Electromagnetic Processes* (Springer, Heidelberg, 1983).
- [4] Yu. L. Klimontovich, *The Kinetic Theory of Non-ideal Plasmas* (Pergamon Press, Oxford, 1982).
- [5] Yu. L. Klimontovich *et al.*, Phys. Rep. **175**, 263 (1989).
- [6] A. G. Sitenko, *Nonlinear Wave Interaction and Fluctuations in Plasma* (Naykova Dumka, Kiev, 1977).
- [7] J. Sheffield, *Plasma Scattering of Electromagnetic Radiation* (Academic Press, New York, 1975).
- [8] T. Koga, *Introduction to Kinetic Theory. Stochastic Processes in Gaseous Systems* (Pergamon Press, Oxford, 1970).
- [9] H. Goldstein, *Classical Mechanics* (Addison-Wesley Press, Cambridge, MA, 1950).
- [10] L. D. Landau and E. M. Lifshits, *Mechanics* (Addison-Wesley Press, Cambridge, MA, 1960).
- [11] G. A. Martynov, Usp. Fiz. Nauk **166**, 1105 (1996).