

Particle swarms in gases: The velocity-average evolution equations from Newton's law

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(Received 11 March 2003; published 11 August 2003)

The evolution equation for a generic average quantity relevant to a swarm of particles homogeneously dispersed in a uniform gas, is obtained directly from the Newton's law, without having recourse to the (intermediary) Boltzmann equation. The procedure makes use of appropriate averages of the term resulting from the impulsive force (due to collisions) in the Newton's law. When the background gas is assumed to be in thermal equilibrium, the obtained evolution equation is shown to agree with the corresponding one following from the Boltzmann equation. But the new procedure also allows to treat physical situations in which the Boltzmann equation is not valid, as it happens when some correlation exists (or is assumed) between the velocities of swarm and gas particles.

DOI: 10.1103/PhysRevE.68.021103

PACS number(s): 05.20.-y, 05.60.-k, 51.10.+y, 51.50.+v

I. INTRODUCTION

In the study of the temporal behavior of a particle swarm in a gas, one often makes use of evolution equations for average quantities (mean velocity, mean energy, etc.). In analogy to what happens for the analogous equations for a simple gas (the so-called equations of change) [1], the above equations are customarily obtained from the Boltzmann equation without trying to get an effective knowledge of its solution (i.e., of the particle distribution). In fact, the evolution equation for the average value $\langle A \rangle$ of the generic (scalar or vector) quantity A is immediately obtained multiplying the Boltzmann equation by A and then integrating over the whole velocity space [2–5]. But, although rather expedient in practice, such a procedure appears to be rather involved and, in a sense, contradictory, from the conceptual point of view. In fact, while the Boltzmann equation was derived (on the basis of the classical laws of particle motion) to explicitly find the time-dependent particle distribution (from which the evolution of any particle velocity average follows immediately), the above procedure seems to have been devised to practically ignore, through the said integration over the velocity space, the details of the form of the evolving, not yet determined, particle distribution. So, it is natural to pose the question: can the evolution equations be directly derived from the Newton's law, without having recourse to the particle distribution function, i.e., to the Boltzmann equation?

From recent studies [6,7] on the motion of large, heavy particles (ions) in gases in external fields, it follows that this question can be affirmatively answered as regards the derivation, in the homogeneous case, of the evolution equation for the particle mean velocity. But a careful consideration of the procedure followed in such studies suggests that the method can be generalized to derive the evolution equation for any average quantity relevant to particles (ions) homogeneously dispersed in a gas in external fields.

The formulation and the discussion of such general method, as well as the discussion on its possible agreement

with the method based on the Boltzmann equation, is the principal—but not the only—aim of this paper. In fact, we shall also put in evidence that our proposed method can be used to obtain results in physical situations to which the Boltzmann theory is inapplicable, as it happens for large, heavy particles in a dense gas [6,7]. For these reasons, the method presented in this paper not only constitutes a conceptual simplification of the theory, but also, we believe, a significant advancement in still rather unexplored areas of the particle kinetic and transport theory.

II. DERIVATION OF THE GENERAL EVOLUTION EQUATION

Consider a swarm of particles (of mass m and number density n) dilutely and homogeneously dispersed in a uniform gas of particles of mass M and number density N . Suppose that every swarm particle is subject to the action of one or more external forces that may also depend on time t and/or on the velocity \vec{v} (but not on the position \vec{r}) of the particle itself. In other words, the swarm particles may be subject to the gravitational force and/or, if they are ions (of charge e), to uniform electric and/or magnetic fields. If we indicate with $\vec{F}(\vec{v}, t)$ the total external force acting on a swarm particle, the Newton's law for such particle is

$$m \frac{d\vec{v}}{dt} = \vec{F}(\vec{v}, t) + \vec{F}_{int}, \quad (1)$$

where \vec{F}_{int} represents the (impulsive) force exerted by the gas particles (through collisions) on the considered swarm particle (of velocity \vec{v}). Obviously, Eq. (1) is the evolution equation for the swarm-particle velocity \vec{v} .

Now, if $A(\vec{v}) \equiv A(v_x, v_y, v_z)$ is a scalar quantity, we can immediately obtain the evolution equation for $A(\vec{v})$ by taking the dot product of Eq. (1) by $\vec{\nabla}_{\vec{v}} A$. In this way we get

$$\vec{\nabla}_{\vec{v}} A \cdot \frac{d\vec{v}}{dt} = \frac{\vec{F}(\vec{v}, t)}{m} \cdot \vec{\nabla}_{\vec{v}} A + \frac{\vec{F}_{int}}{m} \cdot \vec{\nabla}_{\vec{v}} A, \quad (2)$$

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which can also be written as

$$\frac{dA}{dt} = \frac{\vec{F}(\vec{v}, t)}{m} \cdot \vec{\nabla}_{\vec{v}} A + \left(\frac{dA}{dt} \right)_{coll} \quad (3)$$

since the last term in Eq. (2) represents the contribution to dA/dt due to the collisions which, for simplicity, will be assumed to be elastic. This way of writing also follows immediately from the fact that, in the absence of external forces ($\vec{F} = \vec{0}$), one must simply (and obviously) have

$$\frac{dA}{dt} = \left(\frac{dA}{dt} \right)_{coll} \quad (4)$$

It must be stressed that Eq. (3) is the evolution equation [for the generic $A(\vec{v})$] which refers to every swarm particle having velocity \vec{v} at time t . But the collisional term $(dA/dt)_{coll}$ is in practice different from zero only when a collision of the swarm particle with a gas particle occurs. Moreover, the various swarm particles undergo collisions with the gas particles at instants of time which are distributed according to the probability law for the survival of a particle without collisions [8]. In addition, the values taken by such a collisional term depend on the particular dynamics of the collision undergone by the swarm particle considered. So, if we want to arrive, *as a first step*, at an evolution equation [for $A(\vec{v})$], which refers to the *average swarm particle of velocity \vec{v}* , we must first of all consider the subgroup of swarm particles (of velocity \vec{v} at time t) whose first collision with a gas particle will take place (at time $t' \geq t$) in a given way, i.e., with a given dynamics. For all the subgroup particles the set of values taken by the function $(dA/dt)_{coll}$ is obviously the same, but each single value of $(dA/dt)_{coll}$ is taken by the various subgroup particles at different instants of time. In other words, all the functions $(dA/dt)_{coll}$ relevant to the different subgroup particles may be obtained by suitable translations of a single function $(dA/dt)_{coll}$ along the time axis. In these conditions, since a subgroup particle suffers (on the average) one collision in a mean time of flight τ , if the number of swarm particles in the subgroup is sufficiently large, we can replace the (ensemble) average of $(dA/dt)_{coll}$ of all the subgroup particles (at time t), with the temporal average of $(dA/dt)_{coll}$, of a single subgroup particle, over a mean time of flight, i.e., with

$$\begin{aligned} \left(\overline{\frac{dA}{dt}} \right)_{coll} &\equiv \frac{1}{\tau} \int_0^\tau \left(\frac{dA}{dt} \right)_{coll} dt = \left(\frac{\Delta A}{\tau} \right)_{coll} \\ &\equiv \frac{1}{\tau} [A(\vec{v}') - A(\vec{v})]. \end{aligned} \quad (5)$$

In writing this equation we have taken into account that the variation ΔA of A (due to collisions) in a time interval of duration τ is only that occurred in the collision suffered by the subgroup particle in such a time interval. So, in Eq. (5),

\vec{v}' is the velocity of the subgroup particle after a collision initiated with velocity \vec{v} . Moreover, the mean time of flight is

$$\tau = \tau(g) \equiv [NQ(g)g]^{-1}, \quad (6)$$

where g is the relative speed between the colliding particles, i.e., $g \equiv |\vec{V} - \vec{v}|$, \vec{V} being the gas-particle velocity before the collision, and

$$Q(g) \equiv \int_0^{2\pi} d\eta \int_0^\pi \sigma(g, \chi) \sin \chi d\chi \quad (7)$$

is the total scattering cross section resulting from the differential cross section $\sigma(g, \chi)$. In Eq. (7) χ and η are the polar angles of vector $\vec{g}' \equiv \vec{V}' - \vec{v}'$ with respect to $\vec{g} \equiv \vec{V} - \vec{v}$, \vec{V}' being the gas-particle velocity after the collision.

Now, remembering that from the momentum conservation in a collision, one has

$$\vec{v}' = \vec{v} - \frac{M}{m+M} (\vec{g}' - \vec{g}), \quad (8)$$

and that in an elastic collision it is $g' = g$, one immediately sees that, *at fixed \vec{v}* , \vec{v}' depends on g , χ , and η (i.e., on χ , η , and \vec{V}). In other words, assigned values of χ , η , and \vec{V} determine a subgroup of swarm particles in the sense intended above.

Returning, at this point, to the problem of obtaining the evolution equation [for $A(\vec{v})$] relative to the *average swarm particle of velocity \vec{v}* at time t , we must now calculate the appropriate ensemble average of $(dA/dt)_{coll}$, which adequately accounts for all the possible collisions experienced by the swarm particles of velocity \vec{v} . Once such an ensemble average is inserted into Eq. (3) in place of $(dA/dt)_{coll}$, the desired evolution equation is obtained.

To reach this goal, we recall first that $(\overline{dA/dt})_{coll}$ [Eq. (5)] is the ensemble (or temporal) average (for a subgroup of particles of velocity \vec{v}) which accounts simply for the fact that the collisions are distributed in time. Then, we observe that the ensemble average of Eq. (5) over all the possible subgroups of particles of velocity \vec{v} , i.e., over all the possible values of χ , η , and \vec{V} , certainly yields the appropriate ensemble average of $(dA/dt)_{coll}$ we were looking for, viz. (indicating with $\langle \dots \rangle_{\chi, \eta, \vec{V}}$ such an average),

$$\begin{aligned} \left\langle \left(\overline{\frac{dA}{dt}} \right)_{coll} \right\rangle_{\chi, \eta, \vec{V}} &\equiv \frac{1}{N} \int_{\vec{V}} \mathcal{F}(\vec{V}, t) d\vec{V} \int_0^{2\pi} d\eta \\ &\times \int_0^\pi \left(\overline{\frac{dA}{dt}} \right)_{coll} P(\chi, \eta) d\chi. \end{aligned} \quad (9)$$

Here

$$P(\chi, \eta) d\chi d\eta \equiv \frac{\sigma(g, \chi) \sin \chi d\chi d\eta}{Q(g)} \quad (10)$$

is the probability of scattering with polar angles between χ and $\chi + d\chi$, and between η and $\eta + d\eta$, and $\mathcal{F}(\vec{V}, t)$ is the gas-particle velocity distribution (which, in principle, could also depend on \vec{v}) obeying the normalization condition

$$\int_{\vec{V}} \mathcal{F}(\vec{V}, t) d\vec{V} = N. \quad (11)$$

Introducing now Eqs. (5), (6), and (10) into Eq. (9), we get

$$\begin{aligned} \left\langle \left(\frac{dA}{dt} \right)_{coll} \right\rangle_{\chi, \eta, \vec{v}} &= \int_{\vec{V}} \mathcal{F}(\vec{V}, t) d\vec{V} \int_0^{2\pi} d\eta \\ &\times \int_0^\pi [A(\vec{v}') - A(\vec{v})] g \sigma(g, \chi) \sin \chi d\chi, \end{aligned} \quad (12)$$

which is the final expression of the appropriate average collisional term to be considered in the $A(\vec{v})$ -evolution equation for the *average swarm particle of velocity* \vec{v} at time t . Such an equation therefore reads [cf. Eq. (3)]

$$\frac{dA}{dt} = \frac{\vec{F}(\vec{v}, t)}{m} \cdot \vec{\nabla}_{\vec{v}} A + \left\langle \left(\frac{dA}{dt} \right)_{coll} \right\rangle_{\chi, \eta, \vec{v}}, \quad (13)$$

with the last term given by Eq. (12).

It remains at this point to deduce the evolution equation for the average value $\langle A(\vec{v}) \rangle_t$, at time t , of the generic quantity $A(\vec{v})$, when *all* the swarm particles are simultaneously considered (at time t), irrespectively of their velocity. To this end one should obviously take the ensemble average, over the whole particle swarm, of Eq. (3), taking into account that, if \mathcal{N} is the total number of the swarm particles, it is

$$\langle A(\vec{v}) \rangle_t \equiv \frac{1}{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} A_i[\vec{v}_i(t)] \quad (14)$$

and consequently,

$$\left\langle \frac{dA}{dt} \right\rangle_t \equiv \frac{1}{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} \frac{dA_i}{dt} = \frac{1}{\mathcal{N}} \frac{d}{dt} \sum_{i=1}^{\mathcal{N}} A_i = \frac{d}{dt} \langle A(\vec{v}) \rangle_t. \quad (15)$$

Of course, the ensemble average of the term relative to the external force [in Eq. (3)] does not present any difficulty. But the direct evaluation of the ensemble average of the collisional term of Eq. (3) is not easy. We observe, however, that, when performing the ensemble average of the evolution equation for $A(\vec{v})$, we can certainly replace the equation relevant to each swarm particle of velocity \vec{v} [i.e., Eq. (3)] with the corresponding equation [Eq. (13)] relevant to the *average* swarm particle of the same velocity \vec{v} . In this way we get

$$\frac{d\langle A \rangle_t}{dt} = \frac{1}{m} \langle \vec{F}(\vec{v}, t) \cdot \vec{\nabla}_{\vec{v}} A \rangle_t + \left\langle \left\langle \left(\frac{dA}{dt} \right)_{coll} \right\rangle_{\chi, \eta, \vec{v}} \right\rangle_t, \quad (16)$$

which is the evolution equation we were looking for.

It must be stressed that our choice of considering a generic scalar quantity $A(\vec{v})$ is both the most simple and the most general one. In fact, the scalar A may be regarded as a component of a vector (or of a tensor). So, if $\vec{C}(\vec{v})$ is a generic vector, i.e.,

$$\vec{C}(\vec{v}) = \sum_{i=1}^3 C_i(\vec{v}) \hat{e}_i, \quad (17)$$

we can write an evolution equation of the form (16) for the average value of each component $C_i(\vec{v})$. Consequently, summing the three equations so written (each one of them multiplied by the corresponding unit vector \hat{e}_i), we obtain the evolution equation for $\langle \vec{C} \rangle_t$, i.e.,

$$\frac{d\langle \vec{C} \rangle_t}{dt} = \frac{1}{m} \langle (\vec{F}(\vec{v}, t) \cdot \vec{\nabla}_{\vec{v}}) \vec{C} \rangle_t + \left\langle \left\langle \left(\frac{d\vec{C}}{dt} \right)_{coll} \right\rangle_{\chi, \eta, \vec{v}} \right\rangle_t, \quad (18)$$

where, obviously, the last term is given by the ensemble average (over the whole swarm), at time t , of Eq. (12) with \vec{C} in place of A . Of course, when $\vec{C} = \vec{v}$, we have the swarm-particle mean-velocity evolution equation

$$\frac{d\langle \vec{v} \rangle_t}{dt} = \frac{1}{m} \langle \vec{F}(\vec{v}, t) \rangle_t + \left\langle \left\langle \left(\frac{d\vec{v}}{dt} \right)_{coll} \right\rangle_{\chi, \eta, \vec{v}} \right\rangle_t, \quad (19)$$

which could also be obtained by averaging directly Eq. (1), and which, for particular choices of $\vec{F}(\vec{v}, t)$ and of $\mathcal{F}(\vec{V}, t)$, has already been discussed in Refs. [6,7].

III. RELATION WITH THE BOLTZMANN EQUATION METHOD

At this point the problem of the agreement between our present results and those following from the Boltzmann equation must be examined.

In Ref. [6] we have considered the mean-velocity evolution [cf. Eq. (19)] of swarm particles, subject to a constant force \vec{F} , in a gas in thermal equilibrium at a temperature T uninfluenced by the swarm-particle motion, so that $\mathcal{F}(\vec{V}, t)$ is, in effect, the Maxwellian equilibrium distribution

$$\mathcal{F}_M(\vec{V}) = N \left(\frac{M}{2\pi kT} \right)^{3/2} \exp\left(-\frac{MV^2}{2kT} \right), \quad (20)$$

k being the Boltzmann constant. In the said reference, we have treated such situation by a procedure which is a particular case of the general method presented here, and we have noticed that, when the Maxwellian interaction is assumed between swarm particles and gas particles, the result coin-

cides with that following from the Boltzmann equation. We have also pointed out there [6] that, for heavy swarm particles in a light gas (Rayleigh gas), whatever the swarm-particle-gas-particle interaction may be, the result also coincides with that following from the Fokker-Planck equation obtainable [9] from the Boltzmann equation under the assumption that the gas-particle velocity distribution is the equilibrium distribution (20). The same conclusions can be reached if the swarm particles are ions subject to electric and magnetic fields (cf. Ref. [7]). However, such conclusions refer only to Eq. (19) when either the Maxwell interaction model or a large swarm-particle-gas-particle mass ratio is considered, and, in addition, the thermal equilibrium of the background gas is assumed. So, at this stage, nothing can be concluded about the general equation (16) in the most general case. On the other hand, the hypothesis of the thermal equilibrium of the background gas [Eq. (20)] is very common in studies of the behavior of charged-particle swarms in gases [5,10], since it permits the linearization of the Boltzmann equation for the swarm particles. Consequently, the said hypothesis is necessarily present in the investigations on the properties of the corresponding (linearized) collision operator. Since one of these properties is essential to study the equivalence between the Boltzmann-equation method and ours, we shall maintain the above hypothesis in our discussion.

In such hypothesis the Boltzmann equation for the velocity distribution $f(\vec{v},t)$ of our swarm particles in homogeneous conditions is

$$\frac{\partial f}{\partial t} + \frac{\vec{F}(\vec{v},t)}{m} \cdot \frac{\partial f}{\partial \vec{v}} = J(f), \quad (21)$$

where

$$J(f) \equiv \int_{\vec{V}} d\vec{V} \int_0^{2\pi} d\eta \int_0^\pi [\mathcal{F}_M(\vec{V}') f(\vec{v}',t) - \mathcal{F}_M(\vec{V}) f(\vec{v},t)] g \sigma(g,\chi) \sin \chi d\chi \quad (22)$$

is the Boltzmann collision integral.

On the other hand, the ensemble average $\langle A(\vec{v}) \rangle_t$ (at time t) of $A(\vec{v})$, over the whole swarm, is now calculated, through $f(\vec{v},t)$, according to the rule

$$\langle A(\vec{v}) \rangle_t \equiv \frac{1}{n} \int_{\vec{v}} A(\vec{v}) f(\vec{v},t) d\vec{v}. \quad (23)$$

So, in order to find the evolution equation for $\langle A(\vec{v}) \rangle_t$, we multiply Eq. (21) by $A(\vec{v})$ and then integrate over the whole velocity space. The result is (cf., for instance, Refs. [2–4])

$$\frac{d\langle A(\vec{v}) \rangle_t}{dt} - \frac{1}{m} \langle \vec{F}(\vec{v},t) \cdot \vec{\nabla}_{\vec{v}} A \rangle_t = \frac{1}{n} \int_{\vec{v}} A(\vec{v}) J(f) d\vec{v}, \quad (24)$$

where all the symbols $\langle \dots \rangle_t$ must be intended in the sense of Eq. (23).

If we put

$$f(\vec{v},t) = f_M(\vec{v}) h(\vec{v},t), \quad (25)$$

where

$$f_M(\vec{v}) = n \left(\frac{m}{2\pi kT} \right)^{3/2} \exp\left(-\frac{mv^2}{2kT} \right) \quad (26)$$

is the Maxwellian (equilibrium) distribution of the swarm particles, we have

$$J(f) = f_M(\vec{v}) I(h) \\ \equiv f_M(\vec{v}) \int_{\vec{V}} \mathcal{F}_M(\vec{V}) d\vec{V} \int_0^{2\pi} d\eta \int_0^\pi [h(\vec{v}',t) - h(\vec{v},t)] \\ \times g \sigma(g,\chi) \sin \chi d\chi, \quad (27)$$

and consequently,

$$\frac{1}{n} \int_{\vec{v}} A(\vec{v}) J(f) d\vec{v} = \frac{1}{n} \int_{\vec{v}} f_M(\vec{v}) A(\vec{v}) I(h) d\vec{v}. \quad (28)$$

On the other hand, if we define the inner product of two functions $\phi(\vec{v})$ and $\psi(\vec{v})$ as

$$(\phi, \psi) \equiv \frac{1}{n} \int_{\vec{v}} f_M(\vec{v}) \phi(\vec{v}) \psi(\vec{v}) d\vec{v}, \quad (29)$$

we can rewrite Eq. (28) as

$$\frac{1}{n} \int_{\vec{v}} A(\vec{v}) J(f) d\vec{v} = (A, I(h)). \quad (30)$$

But, for the symmetric property of the operator I (see Ref. [11]), we have [cf. Eqs. (25), (27), and (29)]

$$(A, I(h)) = (h, I(A)) = \frac{1}{n} \int_{\vec{v}} f_M(\vec{v}) h(\vec{v},t) I(A(\vec{v})) d\vec{v} \\ = \frac{1}{n} \int_{\vec{v}} f(\vec{v},t) d\vec{v} \int_{\vec{V}} \mathcal{F}_M(\vec{V}) d\vec{V} \int_0^{2\pi} d\eta \\ \times \int_0^\pi [A(\vec{v}') - A(\vec{v})] g \sigma(g,\chi) \sin \chi d\chi. \quad (31)$$

Hence, from Eqs. (30) and (31), by comparison with Eq. (12) [with $\mathcal{F}_M(\vec{V})$ in place of $\mathcal{F}(\vec{V},t)$], and taking into account the definition of ensemble average (23), we have

$$\frac{1}{n} \int_{\vec{v}} A(\vec{v}) J(f) d\vec{v} = \left\langle \left\langle \left(\frac{dA}{dt} \right)_{coll} \right\rangle_{\chi, \eta, \vec{V}} \right\rangle_t. \quad (32)$$

So, Eq. (24) becomes exactly Eq. (16).

Therefore, when the background gas is in thermal equilibrium, our procedure and that based on the Boltzmann equation must be considered equivalent. This is not a surprising result if one considers that the main hypotheses at the ground of the derivation of the Boltzmann equation are in some way contained in our procedure [and in Eq. (20)]. In fact, (1) the

collisions have been tacitly assumed to be binary; (2) the collisional term in Eq. (16) has been evaluated supposing, tacitly, that the collision dynamics is not influenced by the external forces; (3) the duration of a collision has been implicitly assumed to be, in general, much smaller than the duration of a free flight between collisions; and (4) spatial and velocity correlations are absent (i.e., the condition of “molecular chaos” is verified). In fact, gas and swarm particles have been assumed to be uniformly distributed in space. On the other hand, the only velocity distribution involved in our procedure is that of the gas particles, and this distribution, in our equivalence proof, has been assumed to be the \vec{v} -independent distribution $\mathcal{F}_M(\vec{V})$ of Eq. (20).

We want to stress, however, that our procedure is, in a sense, more general than that based on the Boltzmann equation. In fact, our procedure allows to consider also \vec{v} -dependent gas-particle velocity distributions, violating, in this way, the hypothesis of molecular chaos implied in the Boltzmann theory. In effect, a case of this type has already been considered by us in Refs. [6,7] where the motion of large, heavy particles in a gas in any regime has been studied, and a shifted Maxwellian distribution centered at $\vec{V} = \xi\vec{v}$ (with $0 < \xi < 1$) has been chosen as $\mathcal{F}(\vec{V})$. With this

choice, proper formulas for mobility, mean-velocity evolution, and conductivity tensor of large, heavy ions in electric and magnetic fields have been obtained [6,7].

IV. CONCLUSIONS

In this paper, starting from the Newton’s law, we have obtained the evolution equation for any average quantity relevant to particles uniformly dispersed in a gas in external force fields.

The method we have used (1) constitutes the simplest and most direct way to deduce the velocity-average evolution equations from the Newton’s law, (2) establishes the correct statistical procedure, i.e., the succession and the type of the averages which have to be performed to arrive at correct results, (3) obtains results which coincide (at least when the background gas is in thermal equilibrium) with those customarily derived from the Boltzmann equation within its limits of validity, and (4) offers the way to achieve results also in situations in which the Boltzmann equation cannot be employed.

We shall return on the last point, with some applications, in a planned future paper.

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