A New Hierarchy System on the Basis of a "Master" Boltzmann Equation for Microscopic Density

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It is shown that Boltzmann's equation written in terms of microscopic density (namely the unaveraged Boltzmann function) has a wider range of validity as well as finer resolvability for fluctuations than the conventional Boltzmann equation governing Boltzmann's function. In fact the new Boltzmann equation for ideal gases has implications as a microscopically exact continuity equation like Klimontovich's equation for plasmas, and can be derived without invoking any statistical concepts, e.g., distribution functions, or molecular chaos. The Boltzmann equation in the older formalism is obtained by averaging this equation only under a restricted condition of the molecular chaos. The new Boltzmann equation is seen to contain information comparable with Liouville's equation, and serves as a master kinetic equation. A new hierarchy system is formulated in a certain parallelism to the BBGKY hierarchy. They are shown to yield an identical one-particle equation. The difference between the two hierarchy systems first appears in the two-particle equation. The difference is twofold. First, the present formalism includes thermal fluctuations that are missing in the **BBGKY** formalism. Second, the former allows us to formulate multi-time correlations as well, whereas the latter is restricted to simultaneous correlation. These two features are favorably utilized in deriving the Landau-Lifshitz fluctuation law in a most straightforward manner. Also, equations

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describing the nonequilibrium interaction between thermal and fluiddynamical fluctuations are derived.

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1. INTRODUCTION

1.1. BBGKY and Klimontovich Formalisms

It is widely known that one of the most systematic methods for describing the statistical behavior of gases in the nonequilibrium state is provided by the so-called BBGKY hierarchy method.⁽¹⁾ This method has its basis in Liouville's equation, which determines evolution of Liouville's density function, a complete specification of the state of an *N*-particle Hamiltonian system of a gas in terms of 6*N* variables in Γ space.

Another density function which can be compared with the Liouville density function in the level of description has been proposed by Klimontovich in connection with plasma kinetic theory.⁽²⁾ The function, which is called the microscopic density, has an explicit expression of the form

$$\hat{f}(z,t) = \sum_{s=1}^{N} \delta[z - z^{(s)}(t)]$$
(1)

where $z = (\mathbf{x}, \mathbf{v})$ denotes a phase-space point, $z^{(s)}(t)$ gives the locus of the sth particle in the phase space, δ is Dirac's delta function, and the summation is over all particles N under consideration. The microscopic density has a favorable feature in comparison with the Liouville density function: The microscopic density is defined in the (six-dimensional) phase space, in contrast to δN space of the Liouville density, and has a definite physical meaning such that the expression

$$\frac{1}{\Delta \mathbf{x} \ \Delta \mathbf{v}} \int_{\Delta \mathbf{x} \ \Delta \mathbf{v}} \mathring{f} \, d\mathbf{x} \, d\mathbf{v}$$

gives the "exact" number density at an instant t in the phase space z. This is an immediate consequence of the fact that each integrated delta function (1) is unity or zero depending on whether the given particle is located inside or outside, respectively, the volume $\Delta \mathbf{x} \Delta \mathbf{v}$.

The governing equation of the microscopic density \mathring{f} has also been derived by Klimontovich⁽²⁾; this is simply a microscopic equation of continuity in the phase space

$$K\tilde{f} \equiv \frac{\partial\tilde{f}}{\partial t} + \mathbf{v} \cdot \frac{\partial\tilde{f}}{\partial \mathbf{x}} + \frac{\mathbf{\dot{F}}}{m} \cdot \frac{\partial\tilde{f}}{\partial \mathbf{v}} = 0$$
(2)

where $\mathbf{\mathring{F}}$ is the force exerted on a particle at (\mathbf{x}, \mathbf{v}) of the phase space and *m* is the mass of the particle. We note here that no statistical processing has been involved in deriving Eq. (2): This is an exact kinematical relation to be held at any instant, expressing no generation or disappearance of particles in the phase space.

1.2. Objective and Justification

Since the microscopic density \hat{f} contains physical information equivalent to the Liouville density function, and Eq. (2) is similarly related to the Liouville equation, it should be possible to construct a hierarchy formalism on the basis of Eq. (2) and \hat{f} in a certain parallelism to the BBGKY formalism. The objective of this paper is to carry out this procedure for classical ideal gases with binary molecular encounters, in a form which allows direct comparison with the BBGKY counterpart.

Effort along this line, however, would not be very worthwhile if it simply resulted in verifying the correctness of the BBGKY formalism from a different approach. Regarding this point, we can show that the formalism proposed here reveals further details the BBGKY formalism cannot cover, reflecting the fact that the present method has a finer resolvability for fluctuations than does the BBGKY formalism. The subtle point out of which this difference emerges lies in a simple mathematical identity;

$$\sum_{s=1}^{N} \delta(z - z^{(s)}(t)] \sum_{s=1}^{N} \delta[\hat{z} - z^{(\hat{s})}(t)]$$

$$= \sum_{s\neq\hat{s}}^{N} \delta[z - {}^{(s)}(t)] \delta[\hat{z} - z^{(\hat{s})}(t)] + \delta(z - \hat{z})$$

$$\times \sum_{s=1}^{N} \delta[z - z^{(s)}(t)] \qquad (3)$$

Let an average, defined properly, be taken over the identity; then along with definition(1) the following equation results:

$$\hat{f}(z)\hat{f}(\hat{z}) = f_{II}(z,\,\hat{z}) + \,\delta(z\,-\,\hat{z})f(z)$$
 (4)

with f and f_{II} defined by

$$f(z) = \overline{f}^{\overline{s}} \tag{5}$$

$$f_{\rm II}(z,\,\hat{z}) = \sum_{s\,\neq\,\hat{s}}^{N} \,\delta[z\,-\,z^{(\hat{s})}(t)]\,\delta[\hat{z}\,-\,z^{(\hat{s})}(t)] \tag{6}$$

If the average is identified with what is employed in the BBGKY formalism, namely with multiplying by the Liouville density function $f_N(z^{(1)},...,z^{(N)})$ and performing integration with respect to variables $z^{(1)},...,z^{(N)}$, the left-hand side of (6) gives the two-particle distribution function defined there, and in the same way, the function f of (5) coincides with the one-particle distribution, namely the Boltzmann function. As is easily seen [for example, see Eq. (26) of Section 3] the second term on the right-hand side of (4) represents a term yielding the thermal agitation. Then expression (4) shows a clear-cut difference in resolvability, in that the fluctuation correlation in the present formalism [the left-hand side of (4)] includes the thermal agitation, which is missing in the BBGKY formalism. This fact implies that, in the new formalism, heuristic reinterpretations of the existing kinetic theory, such as invoking the Boltzmann–Lengevin equation⁽³⁾ to retrieve thermal agitation, are no longer necessary and are replaced with a direct manipulation. (See Section 3.)

1.3. A Key Version

In dealing with plasmas, namely phenomena associated with Coulomb interactions (soft collisions), the Klimontovich equation (2) is successfully utilized as the master kinetic equation out of which the equation for each level of the hierarchy is derived in a tractable form. This equation, however, is not convenient in dealing with an ideal gas, in which molecular encounters obey the hard collision condition. In fact, the force \mathbf{F} exerted on the molecule would be of the form of a delta-like function having a small width of collision time t^* . Therefore our task is to reformulate the microscopic continuity equation in a form free from the delta-function-like force without degrading the level of description, namely without recourse to any statistical concepts.

1.4. Brief Account of the Approach

Derivation of the master kinetic equation along the line meeting the above requirement is attempted in Section 2. It turns out that the prospective master equation has the form of the Boltzmann equation. It cannot be overemphasized that *this* Boltzmann equation differs from the conventional Boltzmann equation in that it governs the microscopic density \tilde{f} (not the Boltzmann function f) and that it involves no statistical processing, such as molecular chaos. The conventional Boltzmann equation is obtained as its moment equation of the lowest order by averaging the equation and by postulating (binary) molecular chaos. In Section 3 equations of the higher stages of the hierarchy are derived and are compared with their BBGKY counterparts. They are shown to be identical in the homogeneous part of the

equations but to differ in that the present hierarchy equations comprise inhomogeneous terms which are attributed to the presence of thermal agitations. In order to check if the thermodynamic fluctuation is included correctly in the present formalism, an attempt is made to derive the Landau– Lifshitz formula for spontaneous stress and heat flow (Section 4). In Section 5 moment equations describing the evolution, in physical space, of turbulent fluctuations in the course of nonequilibrium interaction with thermal agitations are derived.

2. "MASTER" BOLTZMANN EQUATION

2.1. Limiting Form of the Klimontovich Continuity Equation

A guideline in reformulating the Klimontovich continuity equation to apply to a gas with hard molecules is the following: As we have seen previously, on the one hand, the vanishing collision time ($t^* = 0$) characterizing the hard collision makes it difficult to employ Eq. (2). On the other hand, however, it enables us to single out effects due to collision as instantaneous, far-reaching effects in velocity space, thereby making it possible to formulate molecular interaction in an integral form instead of a divergence form.

Figure 1 illustrates the loci of particles in a binary encounter for (a) hard and (b) soft collisions, respectively. A salient feature of the collision of type (a) is that a particle (say P) that lies on a three-dimensional hyperplane $(\mathbf{x} = \text{const}, \mathbf{v}; \text{arbitrary})$ at time t can reach a specified volume Δz located at (\mathbf{x}, \mathbf{v}) instantly upon collision provided that velocity $\hat{\mathbf{v}}'$ of the collision partner \hat{P} satisfies the conditions

$$\hat{\mathbf{v}}' + \mathbf{v}' = \hat{\mathbf{v}} + \mathbf{v}, \qquad \hat{\mathbf{v}}'^2 + \mathbf{v}'^2 = \hat{\mathbf{v}}^2 + \mathbf{v}^2$$
 (7)

where v' is the velocity of the particle P before collision and where the velocity v of the particle P after collision has been prescribed. Then the change in the number of particles in the volume Δz during the time interval Δt , namely

$$(\partial/\partial t) \int_{\Delta z} \mathring{f} dz \ \Delta t \tag{8}$$

depends on two fluxes, the convective flux Q across the surfaces $\mathbf{x} = \text{const}$ and $\mathbf{x} + \Delta \mathbf{x} = \text{const}$, and the collisional flux P reaching instantly from any part of the hyperplane in a manner analogous to the radiative flux in physical space.

The peculiarity of the present problem, namely the vanishing collision time, lies in the fact that convective flux is allowed only across the surfaces $\mathbf{x} = \text{const}$ and $\mathbf{x} + \Delta \mathbf{x} = \text{const}$ of the six-dimensional volume Δz , whereas



Fig. 1. Schematic representation of six-dimensional (x, v) space and of molecular encounters for (a) hard and (b) soft collisions.

the "radiative" flux is permeable only across the surfaces $\mathbf{v} = \text{const}$ and $\mathbf{v} + \Delta \mathbf{v} = \text{const}$; the two fluxes are apparently discernible because they are *perpendicular* to each other. No such distinction is possible in the case of a soft collision, e.g., Coulomb interaction (Fig. 1b). The first contribution amounts to

$$-(\partial/\partial \mathbf{x}) \cdot \int_{\Delta z} \mathbf{v} \tilde{f} \, dz \, \Delta t \tag{9}$$

and the second one is expressed by a difference of integrals spanning the whole hyperplane, counting the number of particles going into and out of the specified volume.

$$\int_{\Omega'} \mathring{f}(z') \mathring{f}(\hat{z}') \, dz' \, d\hat{z}' \, - \int_{\Omega} \mathring{f}(z) \mathring{f}(\hat{z}) \, dz \, d\hat{z} \tag{10}$$

In the above expression Ω' and Ω are integral regions of the collision partners (z', \hat{z}') and (z, \hat{z}) , respectively, which are located between the hyperplanes $\mathbf{x} = \text{const}$ and $\mathbf{x} + \Delta \mathbf{x} = \text{const}$ and subject to additional conditions (7) and the condition that the collision partners are to collide within time interval Δt . In expression (10), we transform variables as

$$dz' d\hat{z}' = d\mathbf{x}' d\hat{\mathbf{x}}' d\mathbf{v}' d\hat{\mathbf{v}}' = d\mathbf{x}_G' d\mathbf{r}' d\mathbf{v} d\hat{\mathbf{v}}$$
(11)

which is easily confirmed in view of the relations

$$\partial(\mathbf{x}', \mathbf{\hat{x}}')/\partial(x_{G}', \mathbf{r}') = 1, \qquad \partial(\mathbf{\hat{v}}', \mathbf{v}')/\partial(\mathbf{\hat{v}}, \mathbf{v}) = 1$$

where $\mathbf{x}_{G'} \left[= \frac{1}{2} (\mathbf{x}' + \mathbf{\hat{x}}') \right]$ and $\mathbf{r}' \left(= \mathbf{x}' - \mathbf{\hat{x}}' \right)$ denote vectors specifying the center of gravity and the relative location of the two particles, respectively. In the similar way we have

$$dz d\hat{z} = d\mathbf{x}_G d\mathbf{r} d\mathbf{v} d\hat{\mathbf{v}}$$

where the quantities \mathbf{x}_G and \mathbf{r} are defined similarly with respect to the unprimed collision partners (z, \hat{z}) . For sufficiently small Δt , we can put $\mathbf{x}_G' = \mathbf{x}_G = \mathbf{x}$. The integral region of \mathbf{r}' , which forms a subspace of Ω' , constitutes a cylindrical shell with height $|\hat{\mathbf{v}}' - \mathbf{v}'| \Delta t$ and with radius b (the impact parameter), standing on a target plane with target particle z' at the center

$$d\mathbf{r}' = 2\pi |\mathbf{\hat{v}}' - \mathbf{v}'| \Delta t \ b \ db = d\mathbf{r}$$

where invariance of the magnitude of relative velocities

$$V = |\mathbf{\hat{v}}' - \mathbf{v}'| = |\mathbf{\hat{v}} - \mathbf{v}|$$
(12)

an immediate consequence of Eqs. (7), has been utilized. Then the integral (10) is rewritten in the form

$$\Delta t \int_{\Delta z} d\mathbf{x} \, d\mathbf{v} \int \left[\hat{f}(\hat{z}') \hat{f}(z') - \hat{f}(\hat{z}) \hat{f}(z) \right] d\mathbf{K} \, d\hat{\mathbf{v}} \tag{13}$$

with

$$d\mathbf{K} = 2\pi V b \ db$$

It should be stressed here that integral expression (10) counts the exact number of pertinent collisions; in other words, no statistical processing, namely no concept of expectation values, nor any hypothesis of molecular chaos, is involved. In fact, the above manipulation was based only on two factors: the exact number density \hat{f} and deterministic Newtonian mechanics.

The equation of continuity, which expresses no generation or disappearance of particles in the phase space, requires that the total change in the number of molecules in the volume Δz during time interval Δt be attributable

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entirely to two origins: gain/loss due to convection (19) and collision (13). We have, then,

$$\frac{\partial}{\partial t} \int_{\Delta z} \hat{f} dz = -\frac{\partial}{\partial \mathbf{x}} \cdot \int_{\Delta z} \mathbf{v} \hat{f} dz + \int_{\Delta z} dz \int [\hat{f}(\hat{z}')\hat{f}(z') - \hat{f}(\hat{z})\hat{f}(z)] d\mathbf{K} d\hat{\mathbf{v}}$$
(14)

Thus we have obtained an ideal gas version of the plasma kinetic equation (2). If, in the above equation, we introduce a formal procedure of dividing Eq. (14) by Δz and taking a limit of $\Delta z \rightarrow 0$, then we have

$$B\tilde{f} \equiv \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}}\right)\tilde{f} - J(\hat{z}|z)[\tilde{f}(z)\tilde{f}(\hat{z})] = 0$$
(15)

with

$$J(\hat{z}|z)[g(z,\,\hat{z})] = \int [g(z',\,\hat{z}') - g(z,\,\hat{z})] \, d\mathbf{K} \, d\hat{\mathbf{v}}$$
(16)

This is simply Boltzmann's equation, written in terms of the microscopic density in place of the Boltzmann function.

In what follows this equation will play the role of a master equation from which a series of hierarchy equations is generated, just in a similar manner that the BBGKY hierarchy is derived from the Liouville equation. For this reason Eq. (15) is referred to as the master Boltzmann equation (MBE) in the following.

The above formulation is exact only for gases with elastic spherical molecules. Classification into two orthogonal fluxes, one written in a divergence form and the other in an integral form of (15), is obscured if the above reasoning is to be extended to include the power force law

$$|\mathbf{F}| \sim r^{-s}$$

of the molecular interaction. In fact, then, both loci P and Q of Fig. 1a have finite curvature on entering the volume Δz and are not perpendicular to each other. If, however, we can choose the size Δx_i of the volume such that it is larger than the radius of curvature in *almost* all collisions, but is smaller than a characteristic length of long-range effects, then the above method is seen still to be valid. Thus the incorporation of the softer collision into the framework of the present formalism is made possible at the risk of degrading the temporal resolution of the MBE: It is not capable of resolving events with time constant smaller than $t^* = r^*/(RT)^{1/2}$, where r^* denotes the characteristic radius of curvature of a particle upon collision. This does not affect, however, the resolution capability of the present formalism with regard to the thermal agitation.

The extended validity of the MBE for softer molecular encounter is only conditional: Limitation arises from the fact that the collision integral does not converge⁽⁴⁾ for

$$s < 3 \tag{17}$$

This implies that, under this condition, we cannot find the proper volume size Δx_i meeting the requirement stated above, thereby making the two fluxes discernible. Thus the condition $s \leq 3$ provides a criterion as to which of the master kinetic equations (2) or (15) is to be employed in the problem.

2.2. Two Methods of Solving the MBE

Because of the "rugged" or discrete structure of the function \tilde{f} , mathematical tools for solving the MBE (15) are limited to either of the following schemes: The first is a direct method in which the distribution of the particles is simulated by the Monte Carlo method, and evolution at subsequent times is determined according to Eq. (15) for a given initial condition specified properly. A most successful application of this method is seen in the study of rarefied gas dynamics. For example, in the shock structure problem the direct Monte Carlo method yields a solution which agrees with experiments better than those obtained by analytical methods. This is because a welldesigned Monte Carlo method utilizes no averaging procedure, nor any concept of a distribution function,⁽⁵⁾ and thereby simulates direct solution of the MBE (15), whereas the analytical methods^(6,7) solve the conventional Boltzmann equation [Eq. (21) below] with the nonequilibrium correction (ψ term) deleted.

The second method of solving the MBE is to replace the function \hat{f} with a continuous function by means of a certain smoothing procedure, e.g., averaging. Standard analytical methods are made available only via this procedure, and the following part of the paper is devoted to the analytical approach by means of averages taken at various statistical levels of description.

2.3. One-Particle Equation. Comparison with Traditional Boltzmann Equation

In order to compare Eq. (15) with the Boltzmann equation in the older formalism, we take the average of Eq. (15), and utilize expressions (4) and (5); then we have

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}}\right) f(z) = J(\hat{z}|z) [f_{\mathrm{II}}(z, \hat{z})]$$
(18)

In deriving the equation, use is made of the fact that the term $\delta(z - \hat{z})f$,

representing thermodynamic fluctuation, and supposed to appear in the collision integral, is seen to have no contribution: Actually we have, for an arbitrary moment function $\beta(\mathbf{v})$,

$$\int \beta(\mathbf{v}) J(\hat{z}|z) [\delta(z - \hat{z})f] d\mathbf{v}$$

= $\delta(\mathbf{x} - \hat{\mathbf{x}}) \int [\beta(\mathbf{v}') - \beta(\mathbf{v})] \delta(\mathbf{v} - \hat{\mathbf{v}}) f(\mathbf{v}) d\mathbf{K} d\mathbf{v} d\hat{\mathbf{v}} = 0$

because the factor $(\beta' - \beta) \delta(\mathbf{v} - \hat{\mathbf{v}})$ vanishes in view of the relationships⁽⁴⁾

$$\mathbf{v}' = \mathbf{v} + \boldsymbol{\alpha}(\boldsymbol{\alpha} \cdot \mathbf{V}), \qquad \hat{\mathbf{v}}' = \mathbf{v} - \boldsymbol{\alpha}(\boldsymbol{\alpha} \cdot \mathbf{V})$$
(19)

where α is a constant vector defined by the first of Eqs. (19) and V has been defined by (12). Then we readily see that Eq. (18) is identical with the one-particle equation in the BBGKY formalism^(1,4,8,9) provided that the average taken in (18) to have f and f_{II} is the same as described in Section 1.3.

Description in terms of the smoothed distribution functions, namely of the Boltzmann function f, the two-point function f_{II} , etc., is unavoidably connected with a difficulty of indeterminacy³: Equation (18) for the oneparticle equation is linked with effects due to two-particle interaction, and the same is true for the two-particle equation, where three-particle interaction intervenes (see Table I, below). To solve the equation, the chain should be terminated at a certain stage by introducing a closure condition. The quality of the theory depends on two factors, the quality of the closure condition adopted and the stage in the hierarchy at which the truncation is effected. A most primitive form of the closure condition was proposed by Boltzmann in 1872, and has been known as the hypothesis of (binary) molecular chaos:

$$f_{\rm II}(z,\,\hat{z}) \,-\, f(z)f(\hat{z}) \,=\, 0 \tag{20}$$

With this closure condition, Eq. (18) is written as

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}}\right) f = J(\hat{z}|z)[f(z)f(\hat{z})]$$
(21)

which is nothing but the Boltzmann equation in its conventional form. It would be self-explanatory, from the above procedure leading to Eq. (21), that the equation is valid only under far more restrictive conditions than Eq. (15).

2.4. Breakdown of Molecular Chaos

The binary molecular chaos hypothesis (20) has reigned in kinetic theory over a century, and has served as a key hypothesis on which the classical

³ Indeterminacy of this kind is inherent in phenomena that are stochastic and nonlinear. For example, we encounter a similar situation in solving the Navier–Stokes equation for turbulent flows.

Boltzmann equation (21) rests. In Ref. 9, however, the region of validity of the molecular chaos hypothesis has been examined critically, leading to the following findings: Let us define by⁴

$$\psi(z, \hat{z}) \equiv f_{\rm H}(z, \hat{z}) - (1 - N^{-1})f(z)f(\hat{z})$$
(22)

a measure for the deviation from molecular chaos. It is shown that leading terms of ψ decay according to a diffusion equation for a gas in equilibrium. In a nonequilibrium (shear flow) situation, the function ψ is shown to die off eventually insofar as the basic flow is stable with respect to a criterion according to hydrodynamic stability theory. For these cases, therefore, there will be not much danger in putting $\psi = 0$ from the beginning. However, if the basic flow is predicted to be unstable according to the stability criterion, ψ is shown to grow drastically. Thus we see that the molecular chaos hypothesis is misleading in unstable flow situations. The crucial point is that the deviation from molecular chaos now at issue is not the one arising from the dense-gas effect, which is of $O(n^{-1})$ (n is the mean number density), or from a spontaneous correlation which survives only a few collisions, but is a result of macroscopic correlation of O(1), which persists over a hydrodynamic length, namely over thousands of mean free paths. The direct connection of nonvanishing ψ with the unstable flow conditions has caused the macroscopic (turbulent) correlation to be incorporated into the framework of the kinetic theory. On the other hand, it has turned out that the traditional Boltzmann equation (21) is invalidated for these cases and is to be replaced with the one-particle equation (18). Closure at the one-particle stage turns out to be incorrect and under these circumstances we should address ourselves to the multiparticle equations.

3. A NEW HIERARCHY SYSTEM

3.1. Two-Point Two-Time Correlation

The Liouville equation, i.e., the master equation of the BBGKY formalism, describes the evolution of the Liouville density function f_N in the space of $(z_1,..., z_N, t)$ following the standard way of description of multiparticle Hamiltonian mechanics. In statistical mechanics it is often more convenient to discuss correlation in a multiparticle, multitime space, i.e., in the space of $[\zeta(a_1),...,\zeta(a_N)]$, where $\zeta(a)$ denotes a seven-dimensional space [z(a), t(a)]. A formalism along this line is made possible by adapting the

⁴ The factor N^{-1} is unimportant in discussing fluid dynamical behavior of ψ , but is inserted in order to fulfill exactly the condition $\int \psi(z, \hat{z}) dz = 0$. (See Section 3.1.)

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MBE in the following manner: Let us denote by $\tilde{f}(a)$ microscopic density in $\zeta(a)$ space and define the Boltzmann operator B(a) by

$$B(a)\hat{f}(a) \equiv \left[\frac{\partial}{\partial t(a)} + \mathbf{v}(a) \cdot \frac{\partial}{\partial \mathbf{x}(a)}\right]\hat{f}(a) - J(\hat{a}|a)[\hat{f}(a)\hat{f}(\hat{a})]$$
(23)

Let us form

$$\Delta \overline{f(b) \ B(a)} \hat{f}(a) = 0 \tag{24}$$

where

$$\Delta f(b) = \mathring{f}(b) - f(b)$$

denotes an instantaneous fluctuation in the number density in $\zeta(b)$ space, i.e. at a phase space point z(b) and at time t(b). Then, after taking the average, we have an equation of the form

$$\begin{bmatrix} \frac{\partial}{\partial t(a)} + v(a) \cdot \frac{\partial}{\partial \mathbf{x}(a)} \end{bmatrix} \overline{[\hat{f}(a)\hat{f}(b)} - f(a)f(b)]$$

= $J(\hat{a}|a)[\overline{\hat{f}(a)\hat{f}(\hat{a})\hat{f}(b)} - \overline{\hat{f}(a)\hat{f}(\hat{a})}f(b)]$ (25)

In view of definition (1) for the microscopic density the quantity $\overline{\hat{f}(a)}\hat{f}(b)$ is decomposed as

$$\tilde{f}(a)\tilde{f}(b) = f_{\rm II}(a;b) + g(a;b)$$
 (26)

where f_{II} and g are the two-point, two-time distribution function and selfcorrelation function defined, respectively, by

$$f_{\rm II}(a;b) = \overline{\sum_{s_a \neq s_b} \delta[z(a) - z^{(s_a)}(t(a))] \delta[z(b) - z^{(s_b)}(t(b))]}$$
(27)

and

$$g(a;b) = \sum_{s=1}^{N} \delta[z(a) - z^{(s)}(t(a))] \delta[z(b) - z^{(s)}(t(b))]$$
(28)

Note that two arguments separated by semicolon (;) mean two points with correlation taken at different times. The physical meaning of $f_{II}(a; b)$ is straightforward; it denotes the two-point probability density of different particles at different times. On the other hand, the self-correlation g(a; b) expresses the probability of finding the same particle at the point z = z(a) and at the time t = t(a) as was located initially, i.e., at t = t(b), at the point z = z(b). As is easily confirmed, the functions $f_{II}(a; b)$ and g(a; b) reduce, in the limit $t(a) \rightarrow t(b)$, respectively, to

$$f_{\rm II}(a;b) = f_{\rm II}(a,b)$$
 (29)

$$g(a;b) = \delta[z(a) - z(b)]f(a)$$
(30)

where $f_{II}(a, b)$ is the two-point, one-time distribution function defined by (6).

Extending expression (3) to a triple product and taking the average, we are led to the following expression for a three-point, two-time distribution function:

$$\hat{f}(a)\hat{f}(\hat{a})\hat{f}(b) = f_{\text{III}}(a, \hat{a}; b) + \delta[z(a) - z(\hat{a})]f_{\text{II}}(a; b)
+ g_{\text{II}}(a, \hat{a}; b) + g_{\text{II}}(\hat{a}, a; b)
+ \delta[z(a) - z(\hat{a})]g(a; b)$$
(31)

with

 $t(a) = t(\hat{a})$

where the following functions have been introduced:

$$f_{\text{III}}(a, \hat{a}; b) = \overline{\sum_{s_a \neq s_b \neq s_a} \delta[z(a) - z^{(s_a)}(t(a))] \delta[z(\hat{a}) - z^{(s_b)}(t(a))]}$$

$$\overline{\times \delta[z(b) - z^{(s_b)}(t(b))]}$$

$$g_{\text{II}}(a, \hat{a}; b) = \overline{\sum_{s_a \neq s_b} \delta[z(a) - z^{(s_a)}(t(a))]}$$

$$\overline{\times \delta[z(\hat{a}) - z^{(s_b)}(t(a))] \delta[z(b) - z^{(s_b)}(t(b))]}$$
(33)

We note here that the function g_{II} has a mixed character of ordinary correlation (between different particles) and of self-correlation, the latter being characterized by two arguments separated by a semicolon. Therefore g_{II} concerns two particles although it is specified by three arguments. Similarly to what led to (30), definition (33) reduces, for $t(a) \rightarrow t(b)$, to

$$g_{\rm II}(a,\,\hat{a};\,b) \to \delta[z(\hat{a}) - z(b)]f_{\rm II}(a,\,\hat{a}) \tag{34}$$

As will turn out later, decomposition formulas (26) and (31) separate out the thermodynamic part designated by the g's from the total fluctuation. The remaining part, i.e., hydrodynamic fluctuation correlations, are given in terms of multipoint correlations:

$$\psi_{II}(a; b) = f_{II}(a; b) - (1 - N^{-1})f(a)f(b)$$
(35)
$$\psi_{III}(a; b; c) = f_{III}(a; b; c) - (1 - N^{-1})(1 - 2N^{-1})f(a)f(b)$$
$$\times f(c) - (1 - 2N^{-1})f(a)\psi_{II}(b; c) - (1 - 2N^{-1})f(b)$$
$$\times \psi_{II}(c; a) - (1 - 2N^{-1})f(c)\psi_{II}(a; b)$$
(36)

These relations are so designed that integrating condition (36) with respect

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to z(c) yields condition (35). This requirement is necessary in order for the error caused by truncation (e.g., $\psi_{III} = 0$) employed at a certain stage not to affect the exactness of the equations prior to that stage.⁽¹⁰⁾ The factors $1 - N^{-1}$, $1 - 2N^{-1}$, etc. are inserted for the conditions

$$\int \psi_{\rm III}(a;b;c) \, dz(c) = 0, \qquad \int \psi_{\rm II}(a;b) \, dz(b) = 0 \tag{37}$$

to be fulfilled. (Note that f_{II} and f obey the respective conditions $\int f_{II}(a; b) dz(b) = (N - 1)f(a)$ and $\int f(a) dz(a) = N$.) Condition (35) reduces, for t(a) = t(b), to (22), as it should.

In order to close the system at two-particle level, let us introduce an assumption of "ternary" molecular chaos,

$$\psi_{\rm III}(a;b;c) = 0 \tag{38}$$

which makes it possible to express the three-particle distribution function via effects due to binary correlation [See Eq. (36).] Then Eq. (25), when conditions (26) and (35) on its left-hand side, and (31), (36), and (38) on its right-hand side, are utilized, yields the following equation:

$$\begin{bmatrix} \frac{\partial}{\partial t(a)} + \mathbf{v}(a) \cdot \frac{\partial}{\partial \mathbf{x}(a)} \end{bmatrix} [\psi(a; b) + g(a; b)]$$

= $J(\hat{a}|a)[f(a)\psi(\hat{a}; b) + f(\hat{a})\psi(a; b) + g_{II}(a, \hat{a}; b)]$
+ $g_{II}(\hat{a}, a; b)] + O(N^{-1})$ (39)

Terms of $O(N^{-1})$ are unimportant in what follows; only the limiting case $N \rightarrow \infty$ with N/V (V is the total volume under consideration) remaining finite need be considered.

3.2. Self-Correlation in Equilibrium Gases

For a gas in equilibrium the leading terms of the hydrodynamic correlation obey a diffusion equation, and so can be shown to die off eventually.⁽⁹⁾ Therefore we may put from the beginning

$$\psi = 0 \tag{40}$$

in Eq. (39). This condition, then, allows us to put

$$g_{II}(a, \hat{a}; b) = f(a)g(\hat{a}; b)$$
 (41)

which follows directly from the initial condition (34) that g_{II} should obey, along with (30) and the general rule that two particles in an equilibrium gas

are uncorrelated if they are so initially. Thus Eq. (39) is written for an equilibrium gas in the form

$$[(\partial/\partial \tau) + \mathbf{v}(a) \cdot \partial/\partial \mathbf{x}(a)]g(a; b)$$

= $J(\hat{a}|a)[f(a)g(\hat{a}; b) + f(\hat{a})g(a; b)]$ (42)

where τ is defined by

$$\tau = t(a) - t(b) \tag{43}$$

which we shall assume as positive in what follows. Equation (42) is in agreement with the one derived on a different basis by Fox and Uhlenbeck,⁽¹¹⁾ Hinton,⁽¹²⁾ and Chappell.⁽¹³⁾ However, it differs from the one due to Montgomery⁽¹⁴⁾ in that the integrand function of the collision integral is symmetric with respect to *a* and *â*. This symmetry is a consequence of the ternary molecular chaos (38) we have employed, which requires implicitly that the particle should experience many collisions in the course of random flight from z(b) to z(a), i.e., during the elapse of time τ . If, instead, we seek self-correlation of a particle for a very short time during which few collisions are effected, we may put, in the collision term of (25),

$$\overline{\mathring{f}(a)\mathring{f}(\hat{a})\mathring{f}(b)} \sim \overline{\mathring{f}(a)\mathring{f}(b)} \overline{\mathring{f}(\hat{a})}$$

In fact, for such a small τ , correlation between *a* and *b* of an identical particle will not be so destroyed as to be comparable with that for a foreign particle \hat{a} . With this decomposition rule [together with (25) and (26)] a self-correlation equation⁽¹⁴⁾ of the form (42), with the first term on the right-hand side lacking, follows. Thus we see that Eq. (42) and that derived in Ref. 16 are for large and for small τ , respectively.

3.3. Two-Point Simultaneous Correlation

Now we turn to constructing an equation that is symmetric with respect to the two space-time points $\zeta(a)$ and $\zeta(b)$. The symmetry with respect to z(a) and z(b) in the distribution function is favorable in comparing the present theory with the BBGKY theory, in which such symmetry is warranted a priori. Such an equation can be obtained simply by adding to Eq. (39) a transposed equation in which the roles of the variables (a) and z(b) are interchanged. If, in the equation, time variables are transformed according to

$$t = \frac{1}{2}[t(a) + t(b)], \quad \tau = t(a) - t(b)$$

we have the following equation:

$$\begin{bmatrix} \frac{\partial}{\partial t} + \mathbf{v}(a) \cdot \frac{\partial}{\partial \mathbf{x}(a)} + \mathbf{v}(b) \cdot \frac{\partial}{\partial \mathbf{x}(b)} \end{bmatrix} [\psi(a; b) + g(a; b)]$$

$$= \mathscr{I}[\hat{a}|a][f(a)\psi(\hat{a}; b) + g_{\mathrm{II}}(a, \hat{a}; b)]$$

$$+ \mathscr{I}[\hat{b}|b][f(b)\psi(a; b) + g_{\mathrm{II}}(a; b, \hat{b})]$$

$$(44)$$

with the operator \mathcal{I} defined by

$$\mathscr{I}[\hat{a}|a]h(a,\,\hat{a};\,b) \equiv J(\hat{a}|a)[h(a,\,\hat{a};\,b) + h(\hat{a},\,a;\,b)]$$
(45)

Special interest lies in the case of simultaneous correlation, $\tau = 0$. Then the equation in which g and g_{II} have been eliminated by means of (30) and (34) reads

$$\begin{bmatrix} \frac{\partial}{\partial t} + \mathbf{v}(a) \cdot \frac{\partial}{\partial \mathbf{x}(a)} + \mathbf{v}(b) \cdot \frac{\partial}{\partial \mathbf{x}(b)} \end{bmatrix} \psi(a, b) - \mathscr{I}[c|a][f(a)\psi(c, b)] - \mathscr{I}[c|b][f(b)\psi(c, a)] = \mathscr{I}[c|a] \{\delta[z(a) - z(b)]f_{II}(a, c)\} + \mathscr{I}[c|b] \times \{\delta[z(a) - z(b)]f_{II}(b, c)\} - \delta[z(a) - z(b)]J[c|a][f_{II}(a, c)]$$
(46)

3.4. Comparison with BBGKY Hierarchy

In Eq. (46) terms on the left-hand side are connected with macroscale correlation, whereas those on the right-hand side (inhomogeneous terms) have a common factor of a delta function, so are seen to represent effects due to thermodynamic fluctuations, which are missing in the BBGKY formalism. If terms on the right-hand side are put to zero, Eq. (46) is in exact agreement with the two-point BBGKY equation^(8,9) (with ternary molecular chaos).

Comparison of the BBGKY with the present hierarchy system is summarized in Table I. The one-particle equations in both formalisms turn out to be identical if by the bar average we mean

$$\bar{\mathring{g}} = \int \mathring{g} f_N^{\dagger} dz^{(1)} \cdots dz^{(N)}$$

as has been identified in Section 1, where f_N^{\dagger} is a certain function symmetric with respect to its N arguments $[z^{(1)}, ..., z^{(N)}]$, but not necessarily obeying the Liouville equation. The two-particle equation in the BBGKY formalism with no closure condition is written in the form

$$\mathscr{L}[\psi, \psi_{\mathrm{III}}] \equiv \left[\frac{\partial}{\partial t} + \mathbf{v}(a) \cdot \frac{\partial}{\partial \mathbf{x}(a)} + \mathbf{v}(b) \cdot \frac{\partial}{\partial \mathbf{x}(b)}\right] \psi(a, b)$$
$$- \mathscr{I}[c|a][f(a)\psi(c, b)] - \mathscr{I}[c|b][f(b)\psi(c, a)]$$
$$- \{J[c|a] + J[c|b]\}[\psi_{\mathrm{III}}(a, b, c)] = 0$$
(47)

BBGKY hierarchy	Present hierarchy
$\underbrace{\int \cdots \int _{N-1} Lf_N = 0^a}_{N-1}$	$\overline{Bf}^{a} = 0^{a}$
$\underbrace{\int \cdots \int }_{N-2} Lf_N = 0^b$	$\overline{\Delta f(a) Bf'(b) + \Delta f(b) Bf'(a)} = 0^{c}$
$ \underbrace{\int \cdots \int}_{N-3} Lf_N = 0 $	$\overline{\sum \Delta f(a) \ \Delta f(b) \ Bf'(c)} = 0 \ (a, b, c; \text{cycl. permut.})$
$Lf_N = 0$ (Liouville)	$B\dot{f} = 0^d$ (master Boltzmann)
	BBGKY hierarchy $ \int_{N-1} Lf_N = 0^a $ $ \int_{N-2} Lf_N = 0^b $ $ \int_{N-3} Lf_N = 0 $ $ Lf_N = 0 \text{ (Liouville)} $

Table I. Comparison of the Present Hierarchy Equations with the BBGKY Counterparts

^b Eq. (47).

° Eq. (48).

^d Eq. (15).

The corresponding equation in the present formalism reads

$$\mathscr{L}[\psi, \psi_{\mathrm{III}}] = \mathscr{I}[c|a]\{\delta[z(a) - z(b)]f_{\mathrm{II}}(a, c)\} + \mathscr{I}[c|b]\{\delta[z(a) - z(b)]f_{\mathrm{II}}(b, c)\} - \delta[z(a) - z(b)] \times J[c|a]f_{\mathrm{II}}(a, c)$$
(48)

If "ternary" molecular chaos ($\psi_{III} = 0$) is imposed on the equation, it reduces to Eq. (46), as it should.

Constructing three- and higher-particle equations in a form that allows direct comparison with each other is rather straightforward: As to the threeparticle case, the equation in the present formalism is given by

$$\frac{\sum_{\substack{a,b,c:\\(\text{cyclic permutations})}} \Delta f(a) \ \Delta f(b) \ B \mathring{f}(c) = 0 \tag{48'}$$

where the summation is over cyclic permutations of the three space-time points (a, b, c), and where the operator B has been defined by (15). As in the two-particle case, this equation contains more information than the corresponding BBGKY equation

$$\int_{N \to 3} \dots \int_{N \to 3} L f_N = 0$$

where L is the Liouville operator, in the sense that Eq. (48') gives three-time correlation in general, and that it includes thermal agitations as forcing terms. It should be noted at this point that ranges of applicability of the two hierarchy systems are not identical: As was discussed in Section 2.1, the present formalism applies only to hard molecules, whereas the BBGKY formalism has no such limitation in principle. The same procedure of generating a hierarchy system on the basis of Klimontovich equation (2), i.e.,

$$\overline{Kf(a)} = 0$$

$$\overline{\Delta f(a) \ Kf(b) + \Delta f(b) \ Kf(a)} = 0$$

$$\overline{\sum_{\substack{a,b,c:\\ (\text{cyclic permutations})} \Delta f(a) \ \Delta f(b) \ Kf(a)} = 0$$

supplements to cover the whole range of intermolecular force laws, and to form a complete set.

4. DERIVATION OF LANDAU-LIFSHITZ FORMULAS

4.1. Moment Expansion of Function g

We present here an illustration that the present formalism gives a correct account of phenomena ascribed to thermal agitation of the gas. We will show that under equilibrium condition $(u_i = 0, \nabla = 0)$ Eq. (42) for self-correlation g yields a system of moment equations out of which the well-known Landau–Lifshitz fluctuation formulas for spontaneous stress and heat flow are derived.⁽¹⁵⁾ For this purpose we expand the function g in a double series of Hermite polynomials as

$$g(a; b) = \omega(a)\omega(b) \sum \frac{Q_{ij,...,lm...}^{(J,K)}}{c^{J+K}J!K!} \mathscr{H}_{ij,...}^{(J)}(a) \mathscr{H}_{lm...}^{(K)}(b)$$
(49)

where c is the isothermal speed of sound $[=(RT)^{1/2}]$, \mathscr{H} is the three-dimensional Hermite polynomial,⁽⁴⁾ and ω is a function defined by

$$\omega(a) = \frac{1}{(2\pi c^2)^{3/2}} \exp\left[-\frac{v(a)^2}{2c^2}\right]$$
(50)

Note that the Hermite polynomials have the property of orthonormality with the weight function ω , so that the expansion coefficients Q are given as

$$Q_{ij,\dots,lm,\dots}^{(J,K)}(\mathbf{x}(a) - \mathbf{x}(b), \tau) = \int c^{J+K} \mathscr{H}_{ij\dots}^{(J)}(a) \mathscr{H}_{lm\dots}^{(K)}(b) g(a, b) \, d\mathbf{v}(a) \, d\mathbf{v}(b)$$
(51)

Each Q of (51) is shown to be of O(n), which is seen from the initial condition

$$[g(a, b)]_{\tau=0} = \delta[z(a) - z(b)]f(a)$$
(52)

When this initial value of g is substituted in Eq. (51) we have the general expression for initial values of the expansion coefficients Q:

$$Q_{ij\dots,lm\dots}^{(J,K)}(\mathbf{x}(a) - \mathbf{x}(b), \tau) = nc^{J+K} \,\delta[\mathbf{x}(a) - \mathbf{x}(b)] \,\delta_{JK} \sum \delta_{il} \,\delta_{jm} \cdots$$
(53)

where the summation is over N! permutations in the subscripts of Kronecker deltas. In particular, we have

$$[Q^{(0,0)}]_{\tau=0} = n \, \delta[\mathbf{x}(a) - \mathbf{x}(b)]$$

$$[n^{-2}Q^{(1,1)}_{i,l}]_{\tau=0} = n^{-1}c^2 \, \delta_{il} \, \delta[\mathbf{x}(a) - \mathbf{x}(b)]$$
(54)

which give the thermodynamic parts of the density and the velocity correlation of fluctuation, respectively. Furthermore, if we take in Eq. (51) the moment function

$$(m/3)^2 c^4 [\mathscr{H}^{(2)}(a) + 3] [\mathscr{H}^{(2)}(b) + 3]$$
(55)

in place of $c^{J+K}\mathcal{H}^{(J)}(a)\mathcal{H}^{(K)}(b)$, we have the pressure fluctuation formula

$$\overline{\Delta p(a) \ \Delta p(b)} = (m/3)^2 \{9c^4 [Q^{(0,0)}]_0 + [Q^{(2,2)}]_0\}$$
$$= p^2 n^{-1} (5/3) \ \delta[\mathbf{x}(a) - \mathbf{x}(b)]$$
(56)

It is easily examined that fluctuation formulas (54) and (56) are in agreement with those found in textbooks of physics. In a similar fashion we can calculate the fluctuation of viscous stress and heat flow: These two quantities are defined, in the language of the kinetic theory, by

$$\begin{aligned} q_{ij,lm}^{(2,2)} &= \int (mc^2)^2 [\mathscr{H}_{ij}^{(2)}(a) - \frac{1}{3} \delta_{ij} \mathscr{H}^{(2)}(a)] [\mathscr{H}_{lm}^{(2)}(b)] \\ &- \frac{1}{3} \delta lm \mathscr{H}^{(2)}(b)] g \ d\mathbf{v}(a) \ d\mathbf{v}(b) \\ q_{i,l}^{(3,3)} &= \int (\frac{1}{2} mc^3)^2 \mathscr{H}_i^{(3)}(a) \mathscr{H}_l^{(3)}(b) g \ d\mathbf{v}(a) \ d\mathbf{v}(b) \end{aligned}$$

where $\mathscr{H}^{(2)}$ and $\mathscr{H}^{(3)}_i$ are Hermite polynomials contracted with respect to two indices appearing in their subscripts.

In view of (51), these relations read, respectively,

$$\begin{aligned} q_{ij,lm}^{(2,2)} &= m^2 [Q_{ij,lm}^{(2,2)} - \frac{1}{3} \, \delta_{ij} Q_{,lm}^{(2,2)} - \frac{1}{3} \, \delta_{lm} Q_{ij}^{(2,2)} + \frac{1}{9} \, \delta_{ij} \, \delta_{lm} Q^{(2,2)}] \\ q_{i,l}^{(3,3)} &= \frac{1}{4} m^2 Q_{i,l}^{(3,3)} \end{aligned}$$

Their initial values are obtained from (53) as

$$[q_{ij,lm}^{(2,2)}]_{\tau=0} = \frac{p^2}{n} \,\delta[\mathbf{x}(a) - \mathbf{x}(b)] \,(\delta_{il} \,\delta_{jm} + \,\delta_{jl} \,\delta_{im} - \frac{2}{3} \,\delta_{ij} \,\delta_{lm})$$
(57)

$$[q_{i,l}^{(3,3)}]_{r=0} = \frac{5}{2} \frac{p^2}{n} RT \,\delta[\mathbf{x}(a) - \mathbf{x}(b)] \,\delta_{il}$$
(58)

4.2. Moment Equations

Substituting (49) into Eq. (42), multiplying the equation by moment function $c^{2J}\mathscr{H}_{ij...}^{(J)}(a)\mathscr{H}_{im...}^{(J)}(b)$, and performing integrals with respect to $\mathbf{v}(a)$ and $\mathbf{v}(b)$, we obtain a series of moment equations for Maxwellian molecules in a manner similar to the 13-moment method⁽⁴⁾:

$$(\partial/\partial\tau)Q^{(0,0)} = (\partial/\partial\tau)Q^{(1,1)}_{i,l} = (\partial/\partial\tau)Q^{(2,2)} = 0$$
⁽⁵⁹⁾

$$(\partial/\partial\tau)q_{ij,lm}^{(2,2)} + 6nBq_{ij,lm}^{(2,2)} = 0$$
(60)

$$(\partial/\partial\tau)q_{i,l}^{(3,3)} + 4nBq_{i,l}^{(3,3)} = 0$$
(61)

where B is a constant related to the viscosity and the thermal conductivity coefficients as follows;⁽⁴⁾

$$\mu = mRT/6B \qquad \lambda = 5mR^2T/8B \tag{62}$$

Solving Eqs. (60) and (61), eliminating B by the use of (62), and employing the initial conditions (57) and (58), respectively, we are led to the following formulas:

$$q_{ij,lm}^{(2,2)} = n^{-1}p^2 \exp(-\tau p/\mu) \,\delta[\mathbf{x}(a) - \mathbf{x}(b)] \\ \times \left(\delta_{il} \,\delta_{jm} + \,\delta_{im} \,\delta_{jl} - \frac{2}{3} \,\delta_{ij} \,\delta_{lm}\right)$$
(63)

$$q_{i,l}^{(3,3)} = n^{-1} p^2 c_p T \exp(-\tau p c_p / \lambda) \,\delta[\mathbf{x}(a) - \mathbf{x}(b)] \,\delta_{il} \tag{64}$$

where $c_p = \frac{5}{2}R$ is the specific heat under constant pressure of a monatomic gas. If, in Eqs. (63) and (64), the factor $e^{-a\tau}$ ($a \gg 1$) is replaced by (2/a) $\delta(\tau)$, we have familiar forms for the Landau–Lifshitz formulas as derived first on purely macroscopic considerations.⁽¹⁶⁾ Thus, use of the kinetic theory, coupled with the 13-moment method, has enabled us to show the exponential decay of temporal correlation in agreement with a general rule of relaxation phenomena.

5. NONEQUILIBRIUM INTERACTION BETWEEN THERMAL AND MACROSCALE FLUCTUATIONS

Derivation of the Landau-Lifshitz formulas, as shown above, on the basis of the present formalism has assured the accuracy of our basic equation (15), and therefore of the general kinetic fluctuation equation (46) in elucidating phenomena associated with thermodynamic fluctuations. We will discuss in what follows how the thermal agitation interacts with other fluctuations in nonequilibrium situations ($\psi \neq 0$). In order to see how thermodynamic fluctuations interact with the macroscopic ones in physical space, we multiply the moment function $\alpha(a)\beta(b)$ on Eq. (46), the kinetic equation governing

the whole fluctuation, and carry out integration with respect to v(a) and v(b); then we have the following expression for the moment equations:

$$\left\langle \left\langle \frac{\mathscr{D}\alpha\beta\psi}{\mathscr{D}t} + \frac{\partial}{\partial x_{k}(a)} \alpha\beta c(a)\xi_{k}(a)\psi + \frac{\partial}{\partial x_{k}(b)} \alpha\beta c(b) \right. \\ \left. \times \psi - \left(\alpha \frac{D\beta}{Dt} + \beta \frac{D\alpha}{Dt} \right) \psi - c(a)\xi_{k}(a) \frac{\partial\alpha}{\partial x_{k}(a)} \beta\psi \right. \\ \left. - c(b)\xi_{k}(b)\alpha \frac{\partial\beta}{\partial x_{k}(b)} \psi \right\rangle \right\rangle_{ab} - \left\langle \left\langle \left\{ \alpha \right\} \beta f(a)\psi(\hat{a}, b) \right\rangle \right\rangle_{a\tilde{a}}^{\dagger} \right\rangle_{b} \\ \left. - \left\langle \left\langle \left\langle \left[\beta\right] \alpha f(b)\psi(a, \hat{b}) \right\rangle \right\rangle_{b\tilde{b}}^{\dagger} \right\rangle_{a} = \delta[\mathbf{x}(a) - \mathbf{x}(b)]G \right\rangle \right.$$
(65)

with

$$G \equiv \frac{1}{2} \langle \langle \{-[\alpha(a)\beta(a)] + [\alpha(a) + \alpha(\hat{a})][\beta(a)] + [\beta(a) + \beta(\hat{a})][\alpha(a)] \} f_{II}(a, \hat{a}) \rangle \rangle_{a\hat{a}}^{\dagger}$$
(66)

where the following abbreviations are employed:

$$\langle Z \rangle_{a} = \int Z \, d\mathbf{v}(a), \qquad \langle \langle Z \rangle \rangle_{a\dot{a}}^{\dagger} = \int Z \, d\mathbf{K}(a, \hat{a}) \, d\mathbf{v}(a) \, d\mathbf{v}(\hat{a})$$
$$[\alpha(a)] = \alpha(a') + \alpha(\hat{a}') - \alpha(a) - \alpha(\hat{a})$$
$$\frac{\mathscr{D}Z}{\mathscr{D}t} = \frac{\partial Z}{\partial t} + \frac{\partial u_{k}(a)Z}{\partial x_{k}(a)} + \frac{\partial u_{k}(b)Z}{\partial x_{k}(b)}$$
$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u_{k} \frac{\partial}{\partial x_{k}}$$
(67)

and

$$\xi_k = c^{-1}(v_k - u_k) \tag{68}$$

In the above formulas, u_k denotes the hydrodynamic velocity.

We expand the function ψ as

$$\psi(a, b) = \omega(a)\omega(b) \sum_{(J,K)=(0,0)}^{(\infty,\infty)} \frac{R_{ij...,lm...}^{(J,K)}}{c^{J+K}J!K!} \mathscr{H}_{ij...}^{(J)}(a)\mathscr{H}_{lm...}^{(K)}(b)$$
(69)

where ω is given by (50) in which v_k/c is replaced by ξ_k of (68). The expansion coefficients R represent correlation functions in physical space, and their evolution equations are obtained from Eq. (65) in which the moment functions (α , β) are chosen as combinations of the following set of polynomials:

$$m, mc\mathcal{H}_i^{(1)}, mc^2\mathcal{H}_{ij}^{(2)}, \text{ and } mc^3\mathcal{H}_i^{(3)}$$

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where *m* is the mass of a particle, and $\mathscr{H}_i^{(3)}$ is the third-order Hermite polynomial with two indices contracted. This exhausts the whole set necessary in the 13-moment level of description.

Let us consider the simplest case of incompressible flow; then expansion (69) starts with (J, K) = (1, 1), and the moment functions up to $\mathscr{H}_{ij}^{(2)}$ suffice to close the equations. In this case the moment of the lowest order is $(\alpha, \beta) = (m, \mathscr{M}_{i}^{(1)})$, and the associated moment equation gives

$$\partial R_{l,l}^{(1,1)} / \partial x_l(b) = 0 \tag{70}$$

where no contribution from the thermal agitation is observed. For moment functions of higher order, however, effects due to the thermal motion make their appearance, and the two-point Navier–Stokes equation corresponding to the choice of moment $(\alpha, \beta) = (m\mathcal{H}_i^{(1)}(a), m\mathcal{H}_i^{(1)}(b))$ reads

$$\frac{DR_{i,l}^{(1,1)}}{Dt} + \frac{\partial u_{i}(a)}{\partial x_{k}(a)} R_{k,l}^{(1,1)} + \frac{\partial u_{l}(b)}{\partial x_{k}(b)} R_{i,k}^{(1,1)} + \frac{\partial R_{i,l}^{(2,1)}}{\partial x_{i}(a)} + \frac{\partial R_{i,l}^{(1,2)}}{\partial x_{l}(b)} - \nu [\nabla^{2}(a) + \nabla^{2}(b)] R_{i,l}^{(1,1)} = \frac{pp_{il}}{\nu n} \delta[\mathbf{x}(a) - \mathbf{x}(b)]$$
(71)

where p_{il} is the stress deviator tensor and ν is the kinematic viscosity. On the right-hand side terms including $R_{i,l}^{(1,1)}$ are neglected because they are smaller by $O(n^{-1})$ than those on the left-hand side. It is seen in Eq. (71) that the inhomogeneous term on the right-hand side arises from the shearing motion of a gas. This term vanishes for a gas in equilibrium, as it should.

In ordinary fluid mechanics the thermal agitation is not the controlling mechanism in triggering turbulence; it is too small $[O(n^{-1}) \sim 10^{-20}]$ to affect macroscopic phenomena under normal conditions. Turbulence initiation is affected more by free-stream turbulence of a wind tunnel or noise, which enter in the formalism as the initial value of $R_{i,i}^{(1,1)}$ and not as inhomogeneous terms. The thermal agitation contributes to generating macroscopic correlations only under hypothetical conditions of a perfectly quiescent windtunnel.

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