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New Properties of a Class of Generalized Kinetic Equations

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We give some properties of a new class of hard-sphere kinetic equations of great generality, introduced earlier by Polewczak. The assumptions used to obtain the general class are very weak, and the equations include not only the standard and revised Enskog equations, but also generalizations thereof that can be expected to yield essentially exact transport coefficients. In particular, there is a natural two-particle realization that is obtained from maximizing the information entropy subject to prescribed two-particle and one-particle probability distribution functions; k-particle analogs for $k > 2$ also naturally follow. We obtain Liapunov functionals for the whole class of equations under consideration and discuss the question of which of these functionals can be expected to play the role of H-functions. We also obtain several more special results that include new lower bounds on the potential part of the H-function for the revised Enskog equation. The bounds are instrumental in obtaining global existence theorems and also imply that the necessary condition for invertibility of the non-equilibrium extension of local activity as a functional of local density is satisfied.

KEY WORDS: Kinetic theory; entropy; H-theorem; local H-theorem; hard-sphere fluid; BBGKY hierarchy; Enskog equation.

1. INTRODUCTION

In this work we give some new properties of a class of hard-sphere kinetic equations of extremely general functional form introduced recently by Polewczak.[1] Special cases include the standard Enskog equation and revised Enskog equation, which have proved to yield extremely useful

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approximations, but also include a class of much broader equations in which the pair correlation function

$$G = \frac{f_2(t, r_1, v_1, r_2, v_2)}{f_1(t, r_1, v_1)\, f_1(t, r_2, v_2)}$$

for "impact" states is assumed to depend upon velocities v_1 and v_2 (as well as r_1 and r_2) in a very general way. (We are using standard notation here—see below for precise definitions.) The generality appears to be sufficiently great to include f_2's that would yield essentially exact transport coefficients.

We exhibit Liaponov functionals $\Gamma(t)$ for a class of equations (we call them generalized Enskog equations) considered by us. These functionals, defined on sets of nonnegative solutions $D \subset L^1$, are monotone functions of time, whose stationary points determine possible equilibria of the system governed by the generalized Enskog equation. Although in the study of asymptotic stability one usually needs some type of continuity of $\Gamma(t)$: $D \to L^1$, we do not require this property here. In the cases of the Boltzmann and for a class of equations that approximate the revised Enskog equations as a limit (see Theorem 1 of Section 4) corresponding $\Gamma(t)$ are lower semicontinuous in the weak topology of L^1. For our purposes a different assumptions on Γ, namely its lower bound, plays an important role in obtaining the estimation [see (39) of Section 4] that implies the weak compactness argument in L^1, so crucial in existence theorems for the generalized Enskog equations. In addition, when a lower bound is uniform for $t \in [0, \infty)$, the above weak compactness argument determines a weakly compact set of L^1 that (formally at least) plays a role of a global attractor for the system, i.e., an absorbing bounded set which all solutions enter as $t \to \infty$, whatever an initial value is. As we shall discuss, this appears to be a case for which the Liapunov functional $\Gamma(t)$ becomes an H-function for a generalized Enskog equation. In Section 4 we study cases for which one can show existence of a lower bound for Γ. Among various results of Section 4, we obtain new lower bounds for the potential part of the H-function for a class of equations that approach the revised Enskog equation as a limit. As shown in ref. 3, these bounds are also important in demonstrating that the necessary condition for invertibility of $z(t, r)$, the nonequilibrium extension of the activity, in terms of local density is satisfied. In Section 5 we obtain a local version of Γ which, in the cases in which Γ is an H-function, can be considered as an analog of the local H-theorem.

We consider a fluid consisting of hard spheres of diameter a and mass m in an external field F/m and in a spatial domain $\Omega \subseteq R^3$. The external field F/m is assumed to be a smooth function of the spatial variable only. Within the context of (exact) kinetic theory the state of the fluid depends upon (among other things) the one-particle distribution function $f_1(t, r_1, v_1)$, which changes in time due to free streaming and collisions. $f_1(t, r_1, v_1)$ represents at time t the number density of particles at point r_1 with velocity v_1. When two particles with positions at r_1 and r_2 collide, their velocities v_1, v_2 take postcollisional values

$$v_1' = v_1 - \varepsilon\langle \varepsilon, v_1 - v_2\rangle, \qquad v_2' = v_2 + \varepsilon\langle \varepsilon, v_1 - v_2\rangle$$

Here, $\langle \cdot, \cdot \rangle$ is the inner product in R^3, and ε is a vector along the line passing through the centers of the spheres at the moment of impact, i.e., $\varepsilon \in S_+^2 = \{\varepsilon \in R^3\colon |\varepsilon| = 1,\ \langle v_1 - v_2, \varepsilon\rangle \geqslant 0\}$. The exact rate of change of the distribution $f_1(t, r_1, v_1)$ is given by the equation

$$\frac{\partial f_1}{\partial t} + v_1 \frac{\partial f_1}{\partial r_1} + F/m \frac{\partial f_1}{\partial v_1} = \iint dr_2\, dv_2\, K_{12} f_2(t, r_1, v_1, r_2, v_2) \tag{1a}$$

where

$$K_{12} f_2 = a^2 \int_{S_+^2} [f_2(t, r_1, v_1', r_2, v_2')\, \delta(r_1 - r_2 - a\varepsilon) - f_2(t, r_1, v_1, r_2, v_2)\, \delta(r_1 - r_2 + a\varepsilon)]\langle \varepsilon, v_1 - v_2\rangle\, d\varepsilon \tag{1b}$$

The density of pairs of particles in collisional configurations is described by the two-particle distribution function f_2. Expressions for the f_n are given and discussed in terms of open and closed systems near the end of Section 3. We note that in the case of the gas considered in a spatial domain $\Omega \neq R^3$, Eq. (1a) with (1b) needs to be supplemented with suitable boundary conditions.

Equation (1a) with (1b) is one way of writing the exact first BBGKY hierarchy equation for a hard-sphere system, for which the matching condition

$$f_2(t, r_1, v_1', r_2, v_2') = f_2(t, r_1, v_1, r_2, v_2) \tag{2}$$

is satisfied for all v_1, v_2 and r_1, r_2 with $|r_1 - r_2| = a^+$, where v_1' and v_2' are post collisional velocities. The matching condition is typically lost when one introduces an approximate f_2 into (1a) and (1b), which become irreversible. The usual way of introducing an approximate f_2 is by expressing it as a functional of f_1 that is assumed to be independent of boundary conditions. For our purposes it is convenient to do this by first writing f_2 in the form

$$f_2(t, r_1, v_1, r_2, v_2) = G(t, r_1, v_1, r_2, v_2)\, f_1(t, r_1, v_1)\, f_1(t, r_2, v_2) \tag{3}$$

We observe next that f_2 and hence G enters the kinetic equation only for arguments that characterize the precollisional conditions of binary hard-sphere impact, i.e., for $r_{12} \equiv |r_1 - r_2| = a^+$ and $\langle v_1 - v_2, \varepsilon \rangle \geqslant 0$. This is obvious for the second f_2 in (1b). The first f_2 is evaluated for primed velocities, but at $r_2 = r_1 - a\varepsilon$, which makes it "precollisional" also. We shall denote G for such precollisional variables as Y.

The way in which one approximates the exact two-particle correlation function G at impact gives rise to the different kinetic equations found in the literature. The Boltzmann equation is obtained by assuming that $Y \equiv 1$ and that the change of $f_1(t, r_i, v_i)$ over a length a for arbitrary t and v_i is negligible, so that $f_1(t, r_i, v_i) \approx f_1(t, r_i + a\varepsilon, v_i)$. This rather trivial choice for Y is adequate in the dilute-gas limit. For more general Y, the dilute-gas limit is achieved when $Y \to 1$. In the homogeneous case (f_1 does not depend on a position) $Y \to 1$ is implied by $na^3 \to 0$. In nonhomogeneous situations, however, $Y \to 1$ is implied by the local mass estimate

$$\int_{B(r,a)} n(t, z)\, dz \to 0 \qquad \text{for} \quad r \in \Omega$$

where

$$n(t, r) = \int_{R^3} f_1(t, r, v)\, dv$$

$B(r, a) = \{z \in \Omega \colon |z - r| \leqslant a\}$ and Ω is a spatial domain defined in Section 2. We observe that in the homogeneous case the local mass estimate is equivalent to $na^3 \to 0$.

An interesting generalization of Boltzmann's equation (in principle adequate to describe the dilute-gas limit no matter how rapid is the spatial change in f_1, and hence in n, on the length scale of particle diameter) follows from making only the assumption $Y \equiv 1$. In the literature this model is found under the name of the Boltzmann–Enskog equation.

In the standard Enskog theory (SET),[4] Y is given by

$$Y^{\mathrm{SET}}(t, r_1, r_2) = g\left(a^+ \,\middle|\, n\left(t, \frac{r_1 + r_2}{2}\right)\right) \tag{4}$$

where $n(t, r)$ is the local density, and $g(r_{12} \mid n)$ is the pair correlation function at particle separation r_{12} in a uniform equilibrium state at density n. In the revised Enskog theory (RET),[5,6] Y is taken to be the "contact value" of the pair correlation function g for a nonuniform system at equilibrium with local density $n(r)$ in which the correlations depend upon $n(r)$ and the excluded volume of the spheres. In particular, there are no correlations between velocities in the system. In this case one can write

$$Y^{\mathrm{RET}}(t, r_1, r_2) = g(r_1, r_2 \mid n(t, \cdot))\,|_{r_{12} = a^+} \tag{5}$$

The term "revised" points to the fact that in the revised Enskog equation g describes correlations of a nonuniform rather than a uniform equilibrium state, so that $g(r_1, r_2 \mid n(\cdot))$ is a functional of $n(r_1)$ rather than simply a function of the uniform density n. In terms of the formal Mayer cluster expansion, g has the form[11]

$$g(r_1, r_2 \mid n(t, \cdot)) = \Theta_{12} \left\{ 1 + \sum_{k=3}^{\infty} \frac{1}{(k-2)!} \int_{\Omega} dr_3 \cdots \int_{\Omega} dr_k \, n(3) \cdots n(k) \, V(12 \mid 3 \cdots k) \right\} \tag{6}$$

where $n(k) = n(t, r_k)$, $V(12 \mid 3 \cdots k)$ is the sum of all graphs of k labeled points which are biconnected when the Mayer factor $f_{12} = \theta_{12} - 1$ is added, $\Theta_{12} \equiv \Theta(|r_1 - r_2| - a)$, and Θ is the Heaviside step function. The Ω is a spatial domain defined in Section 2.

Finally, following the work of Polewczak,[1] one obtains a new major generalization of the above models by allowing velocity dependence on v_1 and v_2 in Y. In this case Y is considered to be of the form

$$Y \equiv Y(t, r_1, v_1, r_2, v_2 \mid \Lambda f_1) \tag{7}$$

In (7), for each fixed $t \geqslant 0$, Λ indicates an operator, possibly nonlinear, acting on f_1, and $\mid \Lambda f_1$ denotes the functional dependence of Y on Λf_1. We observe that the form of Y in (7) is general enough to include possible functional dependence on f_1 for times prior to t. Typically, Λ represents one or more velocity moments of f_1 [although spatial moments are not excluded in (7)], e.g., the zeroth moment in the cases of the SET and the RET ($\Lambda f_1 = n$). We will assume throughout the paper that Y is nonnegative for $f \geqslant 0$, and that for a fixed but otherwise arbitrary t, Y satisfies the following symmetry restriction:

$$Y \quad \text{is symmetric under} \quad r_1, v_1 \rightleftarrows r_2, v_2 \tag{8}$$

This is precisely the property (8) that is responsible for the existence of a Liapunov functional in the case of the generalized Enskog theory (GET), i.e., Eq. (1a) with (1b) with the closure relation (3) and Y as in (7). This functional has the property $d\Gamma(t)/dt \leqslant 0$, but, in general, this is not enough to imply an approach to true equilibrium. (See the remarks in the first paragraph of Section 4). By recalling the definition of the unit vector ε, we note that $\langle v_1 - v_2, \varepsilon \rangle \geqslant 0$ itself is invariant under the exchange of variables $r_1, v_1 \rightleftarrows r_2, v_2$. Furthermore, the restrictions in (8) under which Y is symmetric are precisely the conditions that are satisfied at the moment of the impact and already used by us in the closure relation (3). We note that in a pioneering paper, the authors of ref. 24 considered an Enskog equation modified by the inclusion of a velocity-dependent correlation function in the collision integral. They did not focus on an H-theorem or related issues, however, and in ref. 24 their main concern was a computation of a correction to the transport coeffiients due to the inclusion of a velocity-dependent correlation function. They approximated Y by a linear-in-velocities perturbation of Y^{SET}.

In general, the exact impact value of G has a functional form that depends upon initial conditions for the ensemble as well as upon t, r_1, v_1, r_2, v_2, and f_1. When Eq. (1a) with (1b) is used to obtain the usual transport coefficients, however, one can assume that memory of the initial conditions is negligible, by definition of the usual transport coefficients. We believe that (7) represents a sufficiently general ansatz so that it includes Y's that will yield transport coefficients arbitrarily close to exact ones. In this paper, and in a companion study[25] of k-particle kinetic equations, $k \geqslant 2$, we discuss an example of a GET that goes beyond the RET and yields a Y of the form given in (7) (see the remarks at the end of Section 3). The GET serves as a formal scheme that appears to embrace all current variants of approximate hard-sphere kinetic equations for f_1 in which quantitative evaluation of such coefficients is tenable.

2. BASIC PROPERTIES OF THE GET

2.1. The Collision Invariants

The generalized Enskog equation, i.e., Eq. (1a)–(1b) with the closure relation (3), Y as in (7), and f_1 replaced by f, can be rewritten in the form

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial r} + F/m \frac{\partial f}{\partial v} = E(f) \equiv E^+(f) - E^-(f) \tag{9}$$

with

$$E^+(f) = a^2 \iint_{R^3 \times S_+^2} Y(t, r, v', r - a\varepsilon, w' \mid \Lambda f) \times f(t, r, v') f(t, r - a\varepsilon, w') \langle \varepsilon, v - w \rangle \, d\varepsilon \, dw \tag{9a}$$

$$E^-(f) = a^2 \iint_{R^3 \times S_+^2} Y(t, r, v, r + a\varepsilon, w \mid \Lambda f) \times f(t, r, v) f(t, r + a\varepsilon, w) \langle \varepsilon, v - w \rangle \, d\varepsilon \, dw \tag{9b}$$

Here, v', w' are the velocities after the collision given by

$$v' = v - \varepsilon \langle \varepsilon, v - w \rangle, \qquad w' = w + \varepsilon \langle \varepsilon, v - w \rangle$$

The first property of $E(f)$ is an analog of the corresponding identity for the Boltzmann collision operator. Property (8) of Y implies that for ψ measurable on $\Omega \times R^3$ and $f \in C_0(\Omega \times R^3)$ we have

$$\iint_{\Omega \times R^3} \psi(r, v)\, E(f)\, dv\, dr$$

$$= \tfrac{1}{2} a^2 \iiiint_{\Omega \times R^3 \times R^3 \times S_+^2} [\psi(r, v') + \psi(r + a\varepsilon, w') - \psi(r, v) - \psi(r + a\varepsilon, w)]$$

$$\times f(t, r, v)\, f(t, r + a\varepsilon, w)$$

$$\times Y(t, r, v, r + a\varepsilon, w \mid \Lambda f) \langle \varepsilon, v - w \rangle\, d\varepsilon\, dw\, dv\, dr \tag{10}$$

We notice that in contrast to the case of the Boltzmann collision operator, for identity (10) to be true we had to integrate over position domain $\Omega \subseteq R^3$. For simplicity, we consider here two cases of spatial domains: $\Omega = R^3$ and a three-dimensional torus, i.e., $\Omega = R^3/Z^3$. The first case (the whole-space problem) will be always considered for systems with finite mass and energy, thus making it different from systems in the whole R^3 which are perturbations from equilibrium near the origin. The second case corresponds to a spatial domain with periodic boundary conditions.

We remark that, because $\int_{R^3} \psi E(f)\, dv \neq 0$ for $\psi = v$ and $\psi = v^2$, the fluid obtained from the GET (including the SET and the RET) does not obey the law of an ideal fluid $p = nkT$, in contrast to the fluid obtained from the Boltzmann equation.

Identity (10) raises the following question: What is a general solution $\psi(r, v)$ in the class of measurable functions on $\Omega \times R^3$ to the functional equation

$$\psi(r, v') + \psi(r + a\varepsilon, w') = \psi(r, v) + \psi(r + a\varepsilon, w)$$

$$\text{for all} \quad r, v, w, \varepsilon \text{ with } \langle \varepsilon, v - w \rangle \geqslant 0 \tag{11}$$

subject to the boundary conditions correspoding to the spatial domains? The answer is known at least for the cases of spatial domains considered above (see ref. 6, pp. 604–605, for a formal proof):

$$\psi(r, v) = h(r) + \langle C_1, v \rangle + C_2 v^2 \tag{12}$$

where $h(r)$ is an arbitrary measurable function defined on Ω, C_1 is a constant vector, and C_2 is a scalar constant. Whether this is true for more general boundary conditions is not clear. Presumably, solutions ψ must be consistent in some sense with given boundary conditions.

2.2. The Liapunov Functionals

For f a nonnegative solution of the generalized Enskog equation, we define

$$\Gamma(t)=\iint_{\Omega\times R^3} f(t,r,v)\log f(t,r,v)\,dv\,dr-\int_0^t I(s)\,ds \tag{13}$$

where

$$\begin{aligned}I(t)=\tfrac{1}{2}a^2\iiiint_{\Omega\times R^3\times R^3\times S_+^2} &[f(t,r-a\varepsilon,w)\,Y(t,r,v',r-a\varepsilon,w'\mid Af)\\ &-f(t,r+a\varepsilon,w)\,Y(t,r,v,r+a\varepsilon,w\mid Af)]\\ &\times f(t,r,v)\langle\varepsilon,v-w\rangle\,d\varepsilon\,dw\,dv\,dr\end{aligned} \tag{14}$$

Now, multiplying the generalized Enskog equation by $1+\log f$ and integrating over $(r,v)\in\Omega\times R^3$, we have

$$\frac{d\Gamma}{dt}=\iint_{\Omega\times R^3} E(f)\log f\,dv\,dr-I(t) \tag{15}$$

Next, using (10) with $\psi=\log f$ together with the inequality $y(\log y-\log z)\geqslant y-z$ for $y,z>0$, we obtain

$$\frac{d\Gamma}{dt}\leqslant 0 \tag{16}$$

The above inequality shows that $\Gamma(t)$ is a Liapunov functional for the problem. Furthermore, as stated in Section 1, when one knows that $\Gamma(t)$ has a lower bound (uniform for $t\in[0,\infty)$), the monotonicity of $\Gamma(t)$ that follows from (16) makes $\Gamma(t)$ a candidate of an H-function for the GET. Indeed, as demonstrated in Section 4 [see (39)], for any solution f of Eq. (9), the uniform lower bound of $\Gamma(t)$ implies the relative weak compactness of the orbit $\{f(t): 0\leqslant t<\infty\}$ in L^1, thus showing that, in principle at least, the minimum of $\Gamma(t)$ (as $t\to\infty$) can be attained. Furthermore, the stationary points of $\Gamma(t)$ are the only minima corresponding to possible equilibria of the system.

We stress that, in general, $\Gamma(t)$ depends on the past of the system governed by Eq. (9). This is in contrast to the H-functions for the Boltzmann as well as the revised Enskog equations, which are functionals of quantities that characterize macrostates at the time t only, i.e., functionals of f itself, and of velocity moments (although, in general, spatial moments are not excluded), evaluated at time t. This last condition together with the monotonicity constitutes the requirements usually imposed on any H-function. The following interesting problem arises: what relations exist between existence of a lower bound for $\Gamma(t)$ (uniform in $t \in [0, \infty)$) and a possible representation of $\Gamma(t)$ in terms of quantities describing macrostates only at time t? In the case of a set of Y's which approach the RET's as a limiting result, Theorem 1 of Section 4 shows that $\Gamma(t)$ is a functional of such quantities only and in the above limiting case reduces to the entropy functional discussed by Résibois[6] and others.[5,8]

We point out that Y in the SET [i.e., Y given as in (4)] satisfies symmetry condition (8), thus showing that the SET has a Liapunov functional. Except in the case of vacuum solutions (see the case 5 of Section 4), which describe the gas escaping from R^3 as $t \to \infty$, and hence with no proper equilibria, the problem of existence of a uniform lower bound for $\Gamma(t)$ in the SET is open, however. We note also that there have been several attempts to find an entropy functional for the SET. Hubert[9] indicated that an H-theorem can be proven for a limited class of functions corresponding to the thermodynamic regime [see the formula (68), p. 89 of ref. 9]. Grmela and Garcia-Colin[10] investigated the role of the symmetric and antisymmetric parts of the standard Enskog collision operator in defining a possible entropy functional. The symmetric and antisymmetric parts were also studied in ref. 9. Neither of these results, however, showed the existence of an H-function for the full collision operator.

Another Liapunov functional can be indicated in the whole-space problem (i.e., when $\Omega = R^3$) and in the absence of an external field ($F \equiv 0$). Multiplying the equation by $(r - tv)^2$, integrating by parts over $r \in R^3$, and using (10) with $\psi = (r - tv)^2$ along with the equality

$$\begin{aligned}(r - tv')^2 &+ (r + a\varepsilon - tw')^2 \\ &= (r - tv)^2 + (r + a\varepsilon - tw)^2 - 2at\langle \varepsilon, v - w\rangle \qquad (17)\end{aligned}$$

for $r, v, w \in R^3$, $t \in R$, $a > 0$, $\varepsilon \in S^2_+$, and v', w' postcollisional velocities, we obtain

$$\begin{aligned}\frac{d}{dt} &\iint_{R^3 \times R^3} (r - tv)^2 f(t, r, v)\, dv\, dr \\ &= -a^3 t \iiiint_{R^3 \times R^3 \times R^3 \times S^2_+} \langle \varepsilon, v - w\rangle^2\, Y(t, r, v, r + a\varepsilon, w \mid \Lambda f) \\ &\quad \times f(t, r, v) f(t, r + a\varepsilon, w)\, d\varepsilon\, dw\, dv\, dr \qquad (18)\end{aligned}$$

In view of (18), the functional defined by

$$\mathscr{E}(t) = \iint_{R^3 \times R^3} (r - tv)^2 f(t, r, v)\, dv\, dr \qquad (19)$$

also indicates dissipativity of the system. In the case of the Boltzmann equation one has $\mathscr{E}(t) = \mathscr{E}(0)$ for all $t \in R$. We observe that $d\mathscr{E}(t)/dt < 0$ only for positive t and nonnegative f. In addition, since identity (17) is true only for the whole-space problem, $\mathscr{E}(t)$ may not be nonincreasing in the case of bounded spatial domain with appropriate boundary conditions. Finally, since $\mathscr{E}(t)$ is decreasing for all times, we see that solutions of the generalized Enskog equation for the whole-space problem cannot approach an absolute Maxwellian.

3. EQUILIBRIUM SOLUTIONS IN THE GET

In spite of the fact that the exact form of the two-particle correlation function is unknown, symmetry property (8) is sufficient to describe the family of all possible solutions for which $d\Gamma(t)/dt = 0$. Indeed, using the fact that $y(\log y - \log z) = y - z$ iff $y = z$, the above family of solutions is characterized by the equality

$$f(t, r, v')\, f(t, r + a\varepsilon, w') = f(t, r, v)\, f(t, r + a\varepsilon, w) \tag{20}$$

for all r, v, w, and ε such that $\langle \varepsilon, v - w \rangle \geqslant 0$. As pointed out by Résibois,[6] the last condition can be relaxed. Following the analysis in ref. 6 together with the requirement that $f(t, r, v)$ be integrable with respect to v, we obtain that the equality (20) is satisfied if and only if

$$f(t, r, v) = n(t, r)[\beta(t) m/2\pi]^{3/2} \exp\{-\beta(t)\, m[v - u(t)]^2/2\} \tag{21}$$

where $u(t)$ is the fluid velocity and $\beta(t) = 1/k_B T(t)$, with $T(t)$ the fluid kinetic temperature. We observe that the form of f in (21) is independent of the choice of Y in (7), and is very different from local equilibrium solutions of the Boltzmann equation, for which u and β can be functions of positions. In the case of the Boltzmann equation the H-function is constant in time if and only if the solution has the form

$$f(t, r, v) = n(t, r)[\beta(t, r) m/2\pi]^{3/2} \exp\{-\beta(t, r)\, m[v - u(t, r)]^2/2\} \tag{22}$$

An example of a solution to the Boltzmann equation in the absence of external forces of the form (22) (albeit one that appears to lack physical significance) is given by

$$f(t, r, v) = c \exp[-b(r - tv)^2], \qquad \text{for some positive constants } c \text{ and } b \tag{23}$$

As is well known, such solutions produce on the hydrodynamic level flows governed by the nondissipative Euler equations of fluid dynamics. The thermodynamic entropy of such systems, if it exists, does not change in time, this being consistent with the fact that on the kinetic level the H-function is constant.

Next we want to analyze the form of solutions to the SET and the RET satisfying (21). By substituting f from (21) in the generalized Enskog equation with Y given by

$$Y = Y(r_1, r_2 \mid n(t)) \tag{24}$$

such that condition (8) is satisfied, we obtain (after integrating with respect to w and ε in the collision operator and comparing coefficients of various powers of v)

$$\frac{\partial \beta}{\partial t} = 0 \tag{25}$$

$$\frac{\partial \log n}{\partial t} - \frac{\beta m}{2} \frac{\partial u^2}{\partial t} + \beta \langle u, F \rangle = -a^2 \left\langle u, \int \frac{\partial \Theta(|r - r_2| - a)}{\partial r} Y(r, r_2 \mid n(t))\, n(t, r_2)\, dr_2 \right\rangle \tag{26}$$

$$\frac{\partial \log n}{\partial r} + \beta m \frac{\partial u}{\partial t} - \beta F = a^2 \int \frac{\partial \Theta(|r - r_2| - a)}{\partial r} Y(r, r_2 \mid n(t))\, n(t, r_2)\, dr_2 \tag{27}$$

where F/m is an external force acting on the system and Θ is the Heaviside step function. Equations (26)–(27) imply the continuity equation

$$\frac{\partial \log n}{\partial t} + u \frac{\partial \log n}{\partial r} = 0 \tag{28}$$

We observe that Eq. (27), for a fixed t, is similar to the first equation of the Born–Green–Yvon equilibrium hierarchy with the external force field $\beta m\, \partial u/\partial t - \beta F$ (see, for example, Chapter 6, Section 33 of ref. 26). This is due to the fact that for hard-sphere potentials the Mayer function appearing in that equation is equal to $\Theta(|r_1 - r_2| - a) - 1$. In the case of the RET, i.e., for Y given by (5), Eq. (27) is precisely the Born–Green–Yvon equation.

Solutions of (26) can be expressed in the form

$$n = \tilde{n}(r) \exp\left(\frac{\beta m}{2} u(t)^2 - \int_0^t \left\langle u(s), \beta F + a^2 \int \frac{\partial \Theta(|r - r_2| - a)}{\partial r} Y(r, r_2 \mid n(s))\, n(s, r_2)\, dr_2 \right\rangle ds \right) \tag{29}$$

where $\tilde{n}(r)$ is a function of position only.

From (21) in the general case of GET or from equations (25)–(29) in the cases characterized by Y given in (24), we conclude that solutions for which a generalization of the H-function is constant are different from solutions obtained under this condition in the case of the Boltzmann equation. Furthermore, the status of the Chapman–Enskog method, which is used to obtain the Navier–Stokes equations and higher-order approximations in the case of the Boltzmann equation, is not entirely clear to us in the case of the GET (including the SET and the RET). A crucial property of the Boltzmann collision operator $Q(f)$, which is used in the Chapman–Enskog method, is the fact that $Q(f)=0$ if and only if f is of the form given in (22). (This is also the only form of the distribution function f for which Boltzmann's H-function can satisfy $dH/dt=0$.) This property is certainly not true in the case of the GET. In fact, except in the trivial case of (21) with $n(t, r)$ being constant, $E(f)\neq 0$. In order to make use of the Chapmann–Enskog method one is forced to expand further the collision operator, corresponding to the SET or the RET, in terms of $a\varepsilon$. This can be justified when the diameter of hard spheres $a\to 0$. From this, and the fact that, as in the case of the Boltzmann equation, the Chapman–Enskog method can be justified asymptotically as the Knudsen number $Kn\to 0$, we conclude that in the case of GET, the Euler equations can be obtained through the Chapman–Enskog method when both the Knudsen number Kn and the diameter a of hard spheres converge to zero. This fact alone introduces various possibilities. Indeed, we can have $Kn\to 0$, $a\to 0$, and at the same time, $a\approx (Kn)^p$ for various $p\geqslant 1$. Presently, one can provide a rigorous proof[33] of the asymptotic convergence of the solutions of the Enskog equation (with Y bounded) to a local maxwellian when $Kn\to 0$, $a\to 0$, and $a\leqslant (Kn)^p$ for $p\gg 1$. Large values of p imply that the diameter a is very small compared to the Knudsen number $Kn\approx l$, where l is a measure of the mean free path. In other words, we are in the range of the dilute-gas limit, where the asymptotic analysis can already be developed on the basis of the Boltzmann equation, rendering a GET analysis of limited interest. In the case of the GET (including the SET and the RET), the physical problem of interest requires the study of the asymptotic convergence in the limit $a\to 0$, $Kn\to 0$, when the diameter a and the Knudsen number Kn are of the same order, i.e., for $p\approx 1$. At present time, the authors are not aware of any compelling arguments, even on the formal level, that provide a resolution of the above problem.

If equilibrium solutions to the problem exist, they can be obtained from Eqs. (25)–(27). Indeed, in this case F cannot depend on time, thus giving equilibrium solutions in the form (21) with $u=0$, $\beta=\text{const}$, and $n(r)$ determined by Eq. (27). In the case of the RET, density $n(r)$ is of the form required by equilibrium statistical mechanics [Eq. (27) is the first Born–

Green–Yvon equation; see ref. 12 for more details]. In general, the specific form taken by Y in Eq. (27) when Y is velocity dependent depends upon the level of approximation being used. An important class of Y's can be provided by the two-particle kinetic theory [see ref. 8, Eq. (63)], where a closure relation this time is supplied for the three-particle distribution function

$$f_3(t, x_1, x_2, x_3) = \frac{f_2(t, x_1, x_2)\, f_2(t, x_1, x_3)\, f_2(t, x_2, x_3)}{f_1(t, x_1)\, f_1(t, x_2)\, f_1(t, x_3)} G_3(t, x_1, x_2, x_3), \qquad x_i = (r_i, v_i) \tag{30}$$

Different choices of G_3 in the above closure relation give rise to different Y's in the following way. Equation (30) can be used in the second BBGKY equation to yield an f_2 which can then be used in (1a)–(1b) to yield an f_1. The resulting $f_2(t, r_1, v_1, r_2, v_2)/f_1(t, r_1, v_1)\, f_1(t, r_2, v_2)$ defines a Y via (3). Among potentially interesting choices of G_3, several stand out as parricularly natural. The simplest is $G_3 \equiv 1$, which corresponds to the Kirkwood superposition approximation (KSA).[24] A very natural choice in terms of the BBGKY hierarchy is to let the function G_3 at an "impact configuration" be given by the same functional of f_1 and f_2 that it is in the case of equilibrium. (The equilibrium G_3 was some time ago shown by Stell[27] to be a functional of f_1 and f_2 that has a formal series representation in the grand ensemble in terms of at-least-triply-connected clusters integrals. In the canonical ensemble, this representation is exact in the thermodynamic limit, but has correction of order N^{-1} for a finite system of N particles.) This is precisely the functional that one will recover in the nonequilibrium case from maximizing the entropy subject to prescribed f_2 (in a closed system with fixed N) or prescribed f_2 and f_1 (in an open system in which one averages over all N), with entropy S given by

$$-S_N/k = (N!)^{-1} \int f_N \log f_N \, d(1) \cdots d(N)$$

in the closed system[28] or $S = \sum_{N \geqslant 0} S_N$ in the open system.[29] Here, we use the notation of $(i) \equiv (r_i, v_i)$ and $d(i) \equiv dv_i \, dr_i$. The appropriate definition of $f_n(1 \cdots n)$ for a closed system is

$$N!/(N-n)! \int f_N(1 \cdots N) \, d(n+1) \cdots d(N)$$

while for an open system it is

$$\sum_{N \geqslant n} \left[N!/(N-n)! \int f_N(1 \cdots N) \, d(n+1) \cdots d(N) \right]$$

We remark that if one uses the f_N generated by the RET (as discussed in ref. 6) to construct an f_3 from these expressions, this f_3 will be the same functional of f_1 and f_2 that the exact f_3 is for a nonuniform system at equilibrium.

Finally, we remark that in the case of the whole-space problem there may not be equilibrium solutions. Indeed, for a large class of initial distributions there are solutions which from the physical point of view describe a fluid that "escapes" from any bounded domain as $t \to \infty$. This has been shown in refs. 13–15 in the case of the Boltzmann equation, and in ref. 16 in the case of a model of the standard and revised Enskog equations. In the GET (with no external forces) the same situation occurs, as indicated by the property of the Liapunov functional $\mathscr{E}(t)$ introduced in Section 2; of particular relevance is Eq. (18).

4. LOWER BOUNDS FOR Γ AND EXISTENCE THEOREMS

In Section 3 we showed the form of solutions for which Γ reaches its stationary value. Next we want to investigate under what conditions Γ is bounded from below. For simplicity of the exposition we assume throughout this section that the external field is absent, i.e., $F \equiv 0$. We remark that the existence of a bound from below (uniform both in time and for the family $\mathscr{F}$ of functions in which one seeks solutions to the problem) does not constitute a sufficient condition for Γ (as a function of f) to reach its minimum value. This is so, in spite of the fact that the function on which Γ can attain its minimum value belongs to the family $\mathscr{F}$. Indeed, in the case of the whole-space problem for the Boltzmann equation (where Γ reduces to the original H-function H_B), Toscani[14] showed that for the solution, f, $H_B(f_\infty) > H_B(M)$, where pointwise $f_\infty = \lim_{t\to\infty} f(t, x+tv, v)$ and M is the Maxwellian (determined by the initial value) on which, by the Gibbs lemma, H_B reaches its minimum [the Gibbs lemma states that among all nonnegative functions f that have the zeroth, first, and second moments constant, the Maxwellian defined by these moments is the only minimum of the functional $H(f) = \int f \log f$]. Since $H_B(f)(t) = H_B(f^{\#})(t)$ for all $t \geq 0$, where $f^{\#}(t, x, v) = f(t(t, x+tv, v)$, we see that $\lim_{t\to\infty} H_B(f)(t) > H_B(M)$ and the solution f does not approach a Maxwellian as $t \to \infty$. This kind of behavior[15] is due to escape of fluid as $t \to \infty$ from any bounded set in R^3 (local rarefication effect). A very similar behavior has been shown for the case of a model of the standard and the revised Enskog equation (with Y assumed to be bounded) in ref. 16. For the solutions obtained in ref. 16 it is easy to see that $|\Gamma(t)|$ is bounded, uniformly in $t \in [0, \infty)$. However, the solution does not approach equilibrium. The above properties of solutions of the Boltzmann or the

Enskog equations also indicate that, in general, the monotonicity of $H_B(t)$ or $\Gamma(t)$ is not sufficient to obtain convergence of solutions to equilibrium. We note that from a physical point of view the asymptotic behavior of solutions, as described above, is not expected from solutions to the problem of gas flow within a container or perturbation from equilibrium in the whole R^3. However, as pointed out by Grad in (ref. 37, p. 259), in the case of the Boltzmann equation "the *H*-theorem gives no indication that there actually will be an approach to absolute equilibrium since it gives no clue to the transition from local to absolute Maxwellian." The problem is, Grad argues (ref. 37, p. 260), "whether the deviation from a local Maxwellian, which is fed by molecular streaming in the presence of spatial inhomogeneity, is sufficiently strong to ultimately wipe out the inhomogeneity." On the other hand, presence of the collisional transfer of momentum and energy implies that the local Maxwellian stage is missing in the GET, as well as in the RET [see (21)]. Thus, we think, the difficulties with an approach to absolute equilibrium, present in the case of the Boltzmann equation, may well be absent in the GET, including the RET. This important topic requires further rigorous study.

Finally, we note that in ref. 6 [see the paragraph before Eq. (49) on p. 603] only a lower bound of Γ (see more remarks on this topic later in the section) has been used in the statement about the existence of a stationary value of the entropy.

We indicate below that lower bounds for Γ play a crucial role in existence theorems for the generalized Enskog equation. We split the Liapunov functional (13) in two parts

$$\Gamma(t) \equiv H_B(t) + H_{corr}(t) \tag{31a}$$

where H_B is the kinetic part of Γ, equal to the usual *H*-function for the Boltzmann equation, and H_{corr} is the part of Γ that describes the effect of correlations. Inequality (16) implies that

$$H_B(t) + H_{corr}(t) \leqslant H_B(0) \tag{31b}$$

Now, the conservation of the mass and the kinetic energy [use (10) with $\psi = 1 + v^2$] implies that for a nonnegative solution of the generalized Enskog equation, $f(t, r, v)$, and for all $t \in [0, \infty)$,

$$\iint_{\Omega \times R^3} (1 + v^2) f(t, r, v)\, dv\, dr = \iint_{\Omega \times R^3} (1 + v^2) f_0(r, v)\, dv\, dr \tag{32}$$

where $f_0(r, v)$ is a nonnegative initial distribution function such that the right-hand side of (32) is finite. Thus, in the case of $\Omega = R^3/Z^3$, the inequality

$$y(\log y - \log z) \geqslant -z \tag{33}$$

with $y = f$ and $z = \exp(-v^2)$ implies that

$$H_{\mathrm{B}}(t) \geqslant -C_{\mathrm{B}} > -\infty \tag{34}$$

uniformly in $t \in [0, \infty)$, where $C_{\mathrm{B}} > 0$ is a constant that depends only on f_0. In the case of the whole-space problem ($\Omega = R^3$), the use of (18) together with rather easy computations given in ref. 1 implies that

$$\sup_{t \in [0,T]} \iint_{R^3 \times R^3} r^2 f(t, r, v)\, dv\, dr \leqslant C_1(T) \tag{35}$$

where $C_1(T)$ also depends on $\iint_{R^3 \times R^3} r^2 f_0\, dv\, dr$ and on $\iint_{R^3 \times R^3} (1 + v^2) f_0\, dv\, dr$. As before, (34), with $y = f$ and $z = \exp(-r^2 - v^2)$, implies that

$$H_{\mathrm{B}}(t) \geqslant -C_{\mathrm{B}}(T) > -\infty \tag{36}$$

Note that in the whole-space problem $C_{\mathrm{B}}(T)$ depends on T. This is partially a reflection of the fact that in this case solutions do not approach an equilibrium (see also a similar remark at the end of Section 2).

Combining all the above, we see that for nonnegative initial data satisfying

$$\iint_{\Omega \times R^3} (1 + v^2 + r^2) f_0(r, v)\, dv\, dr \leqslant C_0 < \infty \tag{37}$$

$H_{\mathrm{B}}(t)$ is bounded from below. We stress that the r^2 term in (37) is superfluous in the case $\Omega = R^3/Z^3$. Now, identity (31a) implies that $\Gamma(t)$ is bounded from below, uniformly on $[0, T]$, if one can show that for $t \in [0, T]$

$$H_{\mathrm{corr}}(t) \geqslant -C_{\mathrm{corr}}(T) > -\infty \tag{38}$$

where $C_{\mathrm{corr}}(T)$ is a positive constant. In the case of periodic boundary conditions a lower bound on $\Gamma(t)$ is uniform on $[0, \infty)$ when the bound in (38) is independent of T. Later in the section, we indicate a class of Y's for which (38) holds uniformly for $t \in [0, \infty)$ in the whole-space problem and in the case of periodic boundary conditions. These Y's approach the RET Y as a limiting case. We point out that Résibois[6] [see the paragraph before Eq. (48) on p. 603 of ref. 6 or the paragraph after inequality (11) on

p. 1410 in ref. 18] stated that $H_{\text{corr}}(t)$ is bounded. However, the arguments given in refs. 6 and 18 are not complete.

Inequality (38), together with (31b), also implies that

$$H_{\text{B}}(t) \leqslant H_{\text{B}}(0) + C_{\text{corr}}(T) \tag{39}$$

uniformly in $t \in [0, T]$, for any $T > 0$. Thus we have proven that for a nonnegative initial distribution f_0 satisfying

$$\iint_{\Omega \times R^3} [1 + v^2 + r^2 + |\log f_0(r, v)|] f_0(r, v)\, dv\, dr \leqslant C_0 < \infty \tag{40}$$

inequality (38) yields the following *a priori* bound for a nonnegative solution $f(t, r, v)$:

$$\sup_{t \in [0,T]} \iint_{\Omega \times R^3} [1 + v^2 + r^2 + |\log f(t, r, v)|] f(t, r, v)\, dv\, dr \leqslant C_T < \infty \tag{41}$$

As before, in the case of periodic boundary conditions ($\Omega = R^3/Z^3$), the r^2 term in (40) and (41) is superfluous.

Estimation (41) places the generalized Enskog equation in the framework of the DiPerna–Lions method[17] developed for the Boltzmann equation. Let us observe that in the case of the Boltzmann equation $H_{\text{corr}} \equiv 0$; thus the bound (38) is trivially satisfied.

A priori estimation (41) has a very important physical interpretation. It implies that there can be no concentration of density in the system, in a sense that inequality (43) below makes precise. [Such concentrations would not be expected in an exact description of a hard-sphere system, except at close packing, since the hard cores prevent particles from overlapping, and only at close packing will the lack of thermal motion lead to the frozen-in configurations characterized by δ-function shells describing $n(t, r)$.] From the fact that

$$\sup_{t \in [0,T]} \iint_{\Omega \times R^3} f(t, r, v) \log f(t, r, v)\, dv\, dr \leqslant C_T < \infty \tag{42}$$

we obtain that the family of densities $\{n(t, r): t \in [0, T]\}$ is uniformly integrable, i.e., to each $\varepsilon > 0$ there corresponds a $\delta > 0$ such that

$$\int_E n(t, r)\, dr < \varepsilon \tag{43}$$

whenever $t \in [0, T]$ and $\text{vol}(E) < \delta$. In other words, (43) implies that there can be no large concentrations of $n(t, r)$ in arbitrary small domains. As before, T can be set to ∞ when the bound in (38) is independent of T. We observe that in the case of the Boltzmann equation a similar bound to (43) follows directly from the H-theorem, while in the GET we needed an additional condition (38) to satisfy (43).

Now we want to indicate several classes of problems for which the bound (38) holds uniformly in $t \in [0, T]$, with $T = \infty$ in some cases. The bound (38), through estimation (41), is intimately related to the problem of finding solutions for the GET. In the proof of existence theorems for the GET,[1] one needs boundedness of Y, in addition to the symmetry condition (8). More precisely, Y in ref. 1 is assumed to be bounded on a set of functions having bounded mass and energy. In this paper, and especially throughout this section, we follow ref. 1 in assuming that Y is bounded. We also indicate a class of problems for which the last condition holds.

Case 1. If the density function $n(t, r)$ is bounded by $C_n(T)$, uniformly in $t \in [0, T]$ and $r \in \Omega$, then (38) is satisfied with a constant $C_{\text{corr}}(T)$ also depending on $C_n(T)$ and $\iint_{\Omega \times R^3} (1 + v^2) \, |f(t, r, v)| \, dv \, dr$.

The proof follows from a simple integration of (14). We observe that even in the case where $n(t, r)$ is bounded uniformly in $t \in [0, \infty)$, and $r \in \Omega$, the bound in (38) may be valid only for finite T. We note that in the spatially homogeneous case, the Mayer cluster expansion (6) is convergent for small enough densities. Therefore, Y's computed in the SET and the RET are bounded, thus implying (38). We believe that (6) should be convergent for small densities also in the nonhomogeneous case, although we cannot provide a rigorous proof of this fact except for densities coming from nonuniform equilibrium systems, following Ruelle (ref. 38, Chapter 4). We stress, however, that even when one is not concerned with the convergence of the series representing Y in the SET or the RET, the argument that uses the boundedness of the density is not complete. Indeed, presently, we do not know in general whether the GET, including the RET and the SET, preserves this property with evolution of time. On the other hand, in the absence of external forces and when the initial value f_0 does not depend on r, the generalized Enskog equation preserves spatial homogeneity with evolution of time, whenever Y is translationally invariant in position. Hence, in the homogeneous case the argument that uses the boundedness of density is a complete one. We also add at this point that in the homogeneous case, the RET and the SET are equivalent ($Y^{\text{SET}} = Y^{\text{RET}}$).

The next case reveals a surprising property, connecting together the kinetic and the correlational parts of Γ for the whole-space problem ($\Omega = R^3$) (see ref. 1, p. 498).

Case 2. Suppose that $f(t, r, v)$ is a mild nonnegative solution of (9) [ref. 1, Eq. (2.12) for the definition of a mild solution] in the case $\Omega = R^3$ with a nonnegative initial distribution f_0 satisfying condition (40). Then the bound (42) implies (38). In fact, (42) is equivalent to the boundedness of $|H_{\text{corr}}(t)|$ uniformly in $t \in [0, T]$ and for any $T > 0$. The above result is true for each bounded and symmetric Y of the form (7).

Case 3. Suppose that $f_0 \geqslant 0$ satisfies (40) with $\Omega = R^3$ (the whole-space problem). If either (a) $0 < T < \infty$ is arbitrary and

$$\| f_0 \|_{L^1(R^3 \times R^3)} \equiv \iint_{R^3 \times R^3} |f_0| \, dv \, dr$$

is sufficiently small (small initial mass) or (b) $T > 0$ is sufficiently small and $\| f_0 \|_{L^1(R^3 \times R^3)}$ is arbitrary, then the bound (38) holds.

This result is essentially contained in Theorem 2.1 of ref. 1. In fact, the main idea of the proof of Theorem 2.1 is based on the fact that $|H_{\text{corr}}(t)|$ is bounded uniformly for $t \in [0, T]$ under either the assumption (a) or (b). The bound depends on T and the constant C_0 in (40). From a physical point of view, the necessity of conditions (a) or (b), in particular when Y depends on velocities, might be expected to follow from the fact that velocity correlations may induce concentrations of the density at later times, even if initially such concentrations were absent. Hence, $|H_{\text{corr}}|$ may become unbounded at such later times [since the negation of (43) implies the negation of (38)]. On the other hand, a small enough initial mass will allow fluid to disperse quickly, even in the presence of velocity correlations, although such correlations can eventually have an effect on the long-time mass distribution. This possible unboundedness of $|H_{\text{corr}}|$ after sufficiently long times is closely related to the fact that in the dilute-gas limit, velocity correlations do not prevent the Boltzmann equation from becoming an increasingly accurate description of transport processes as one approaches the dilute-gas limit, despite the fact that the correlations can make themselves felt on sufficiently long time scales for arbitrarily small na^3. In particular, the Boltzmann-equation expressions for transport coefficients become exact when $\Omega = R^3$ as $na^3 \to 0$, although slowly decaying velocity correlations result in coefficients that are nonanalytic in n about $n = 0$.[30]

Another interesting case of (38) is provided by the whole-space problem with the grazing collisions removed from the scattering kernel of $E(f)$: We have the following situation.

Case 4. Suppose that f_0 satisfies condition (40) and for some $\gamma > 0$ the scattering kernel $\langle \varepsilon, v - w \rangle$ in $E(f)$ is replaced by

$$\chi_\gamma \times \langle \varepsilon, v - w \rangle$$

Here χ_γ is the characteristic function of the set $\{(\varepsilon, v, w) \in S_+^2 \times R^3 \times R^3: \langle \varepsilon, v-w \rangle \geqslant \gamma\}$ and $\gamma > 0$ is arbitrary small. Then the bound (38) holds and is independent of time. On the other hand, because of (36), the lower bound on $\Gamma(t)$ depends on T, for $T > 0$ arbitrary but finite. Inequality (18) for the functional $\mathscr{E}(t)$, defined in (19), plays a crucial role in the proof. From a physical point of view it means that we eliminate collisions (called the grazing collisions) that result in small changes of v' and w' as compared with their precollisional values v and w, respectively. We point out that a similar cutoff has been common in the case of the Boltzmann collision operator. Indeed, the restriction of the deflection angle θ to $0 \leqslant \theta \leqslant \pi/2 - \gamma$ for some small $\gamma > 0$ results in elimination of the grazing collisions. We remark, however, that the angular cutoff in the case of the Boltzmann equation was needed to handle a singularity resulting from an infinite range of interactions of the inverse power potentials. Here, since we consider only hard spheres, such a singularity does not appear. For technical reasons, however, we still need the truncation in the scattering kernel to obtain an existence result global in time with an arbitrary initial mass and bounded Y of the form (7).

For the vacuum solutions, already mentioned in the beginning of this section, we have the following case.

Case 5. Suppose that $f(t, r, v)$ is a nonnegative vacuum solution obtained in refs. 31 and 16 in the case of a bounded Y that is independent of velocities [for example, of the functional form as in (4) or (5)]. Then (38) holds. In fact, one can show that $H_{\text{corr}}(t)$ is bounded uniformly in $t \in [0, \infty)$. It is worth pointing out that vacuum solutions obtained in ref. 31 can have infinite mass and be singular in velocities.[32]

In the points 1–5 presented above, we have considered various conditions imposed either on initial states (points 3 and 5), or on the range of possible collisions (point 4). In point 1, the *a priori* bound on density $n(t, r)$ was enough for (38) to hold. A particular form of Y, except, of course, for the symmetry and boundedness, did not play any role in establishing (38) in 1–5. With regard to points 1–5, there are two notes of criticism. First, the conditions imposed in 1–5 are usually of very restrictive nature, in particular, when one seeks solutions global in time with arbitrary initial mass. Second, Y's in the SET and the RET are of very special form [see (4)–(6)], not yet accounted for, in points 1–5. It is therefore important to consider a class of problems that would be free of the above criticism.

For $i \geqslant 2$ consider G of the form

$$G = \Theta_{12} \left\{ 1 + \sum_{k=3}^{i} \frac{1}{(k-2)!} \int_\Omega dr_3 \cdots \int_\Omega dr_k \, n(3) \cdots n(k) \, V(12 \mid 3 \cdots k) \right\} \quad (44)$$

with the same notation as in (6) and with the convention that $G=\Theta_{12}$ for $i=2$. The case $i=2$ corresponds to the Boltzmann–Enskog equation, i.e., the case when $Y\equiv 1$. We remark that, except for $i=2$ and $i=3$, we cannot prove that the contact value Y obtained from G in (44) is nonnegative for $f\geqslant 0$. This property, however, is not required in Theorem 1 and Corollary 2 below. Let $u(t, r)$ be the fluid velocity defined by

$$n(t, r)\, u(t, r)=\int_{R^3} vf(t, r, v)\, dv \tag{45}$$

We have the following result.

Theorem 1. Suppose that $(1+|v|)\, f(t, r, v)$ and $(1+|v|)(\partial f/\partial r)(t, r, v)$ are integrable over $[0, T]\times\Omega\times R^3$ and such that

$$\frac{\partial n}{\partial t}+\frac{\partial(nu)}{\partial r}=0 \tag{46}$$

Then for Y, obtained from G given in (44), the following identity holds:

$$H_{\text{corr}}(t)=-\int_\Omega n(t, r_1)\, S_{\text{corr}}(t, r_1)\, dr_1+\int_\Omega n(0, r_1)\, S_{\text{corr}}(0, r_1)\, dr_1 \tag{47}$$

where

$$S_{\text{corr}}(t, r_1)=\sum_{k=2}^{i}\frac{1}{k!}\int_\Omega dr_2\cdots\int_\Omega dr_k\, n(2)\cdots n(k)\, V(1\cdots k) \tag{48}$$

and $V(1\cdots k)$ is the sum of all irreducible Mayer graphs which doubly connect k particles.

Sketch of the Proof. Following the ideas similar to those presented in refs. 7 and 22 [in particular, Eqs. (14)–(18) of ref. 7 and (3.17)–(3.19) of ref. 22] and using (46), the symmetries of $V(12\mid 3\cdots k)$ and $V(1\cdots k)$, and the translational invariance of G in (44)

$$G(r_1+r, r_2+r\mid n(t,\cdot))=G(r_1, r_2\mid n(t,\cdot+r)),\qquad \text{for any}\quad r\in\Omega \tag{49}$$

one obtains the equation for $H_{\text{corr}}(t)$:

$$\frac{d}{dt}H_{\text{corr}}(t)=-\frac{d}{dt}\int_\Omega n(t, r_1)\, S_{\text{corr}}(t, r_1)\, dr_1+\int_\Omega\frac{\partial\Phi}{\partial r_1}(t, r_1)\, dr_1$$

Here, $\Phi(t, r_1)$ is some multilinear function of n and nu, with the dependence on t and r_1 only through n and nu. This, together with the integrability assumptions of $(1 + |v|) f(t, r_1, v)$ and $(1 + |v|)(\partial f/\partial r_1)(t, r_1, v)$, implies that the second term on the right-hand side of the last equation is zero, thus yielding Eq. (47).

We observe that (47) holds for $f(t, r, v)$ that are not necessarily solutions of the corresponding Enskog equation [with Y obtained from G given in (44)], as long as they satisfy the continuity equation (46). We also remark that (47), combined with (13) and (31a), implies that $dH_{corr}(t)/dt = I(t)$, i.e., for Y obtained from G as in (44), the dependence of $\Gamma(t)$, defined in (13), on times prior to time t is superficial. Formally, (47) holds also for $i = \infty$, and in this case S_{corr} has the functional form of the correlational entropy density for hard spheres at equilibrium (see, for example, ref. 11). Furthermore, for $i = \infty$, G in (44) becomes the pair correlation function in a nonuniform equilibrium state at density n, thus being nonnegative for $f \geqslant 0$. We recall that $V(12) = f_{12}$ and $V(123) = f_{12} f_{23} f_{13}$, where f_{ij} is the Mayer function between particles i and j. For $V(1 \cdots k)$ with $k \geqslant 4$, see, for example, ref. 11. On the same purely formal level, the one-particle Liapunov functional generated by the G_3 described at the end of Section 3 can be shown to have the functional form given by (48) (with $i = \infty$), but with the Mayer function replaced by a velocity-dependent generalization, as described below Eq. (4) in ref. 39, and in detail in ref. 25. Because this representation manifestly involves only quantities evaluated at time t, it gives rise to a Liapunov functional that depends on functions describing a microstate at the same time t only, just as in the case of the RET.

Ultimately one would like to consider rigorously the case of $i = \infty$ in (44); the fact that Theorem 1 holds for any finite i seems to us to be a very promising result in this direction, going considerably beyond previous treatments.

Corollary 2. Suppose that $f(t, r, v)$ satisfies the conditions of Theorem 1. Then for all $t \in [0, T]$

$$|H_{corr}(t)| \leqslant C(i) \sum_{k=2}^{i} \left(\|f(t)\|^k_{L^1(\Omega \times R^3)} + \|f(0)\|^k_{L^1(\Omega \times R^3)} \right) \tag{50}$$

where

$$\|f(t)\|_{L^1(\Omega \times R^3)} = \iint_{\Omega \times R^3} |f(t, r, v)| \, dv \, dr$$

The proof of Corollary 2, for each $i \geqslant 2$, follows immediately from Theorem 1 after simple integrations of (48) with respect to $dr_2 \cdots dr_k$ for $2 \leqslant k \leqslant i$. It is important to observe that for each $i \geqslant 2$, $C(i)$ does not depend on T.

The result of Corollary 2 gives the bound (38) for H_{corr}. Its use in providing the estimation (41), needed in existence theorems, or a lower bound for $\Gamma(t)$, is limited to the cases for which the contact value Y obtained from G in (44) is nonnegative for $f \geqslant 0$. As noted earlier, except for $i=2$ and $i=3$, we cannot prove that this condition is true for $i \geqslant 4$. We have the following situation.

Case 6. Suppose that $f_0 \geqslant 0$ satisfies (40) and consider Y obtained either from G given in (44) for $i=2$ or $i=3$. Then $\Gamma(t)$ is bounded from below, uniformly for $t \in [0, T]$. Furthermore, in the case of periodic boundary conditions, (34) implies that a lower bound of $\Gamma(t)$ is uniform for $t \in [0, \infty)$.

We observe that point 6 provides a class of Y's which are bounded. Furthermore, in contrast to points 1–5, such Y's imply that $\sup_{t \in [0,\infty)} |\Gamma(t)|$ is finite in the case of periodic boundary conditions.

The next theorem[2] is a basic existence result for the generalized Enskog equation with Y given in point 6.

Theorem 3. Assume that $\Omega = R^3/Z^3$ or $\Omega = R^3$ and that $f_0 \geqslant 0$ satisfies (40). Then for each $T > 0$ there exists $f(t, r, v)$ for which condition (41) holds and such that for almost all $(r, v) \in \Omega \times R^3$

$$f^{\#}(t, r, v) - f^{\#}(s, r, v) = \int_s^t E(f)^{\#}(\lambda, r, v)\, d\lambda, \qquad 0 < s < t \leqslant T \quad (51)$$

where $E(f)$ is the generalized Enskog collision operator with Y given in point 6, and $f^{\#}(t, r, v) = f(t, r + tv, v)$.

We note that the case $i=3$ of Theorem 3 extends the result of $Y=1$ (i.e., when $i=2$) previously obtained by Arkeryd,[34] Esteban and Perthame,[35] and Arkeryd and Cercignani.[36] Furthermore, it can be shown in a similar way to the proof of the original result that an analog of Theorem 1, and ultimately Corollary 2 and Theorem 3, holds for any finite i when all nonnegative terms [i.e., the terms containing odd numbers of the Mayer functions in $V(12 \mid 3 \cdots k)$] are removed from G in (44).

We end this section with some further implications of bound (42) [a consequence of (38)] for the inverse problem that arises naturally in the density functional approach in the theory of nonuniform fluids.[19,20] In particular, this approach has been used in ref. 6 to derive formally the revised Enskog equation from a special grand canonical ensemble. The crucial assumption in the density functional approach, as well as in the Résibois derivation, is that every density $n(\cdot)$, which is the symmetrized one-particle reduction of a probability distribution function, is an equilibrium one-particle density at some external potential $U(\cdot)$. This is the inverse problem, also equivalent to the existence of the map $n(\cdot) \mapsto U(\cdot)$. If such a map exists, then $U(\cdot)$ becomes a functional of $n(\cdot)$. Thus, the activity function $z(\cdot)$ introduced in ref. 6, $z(\cdot) \rightleftharpoons \exp[-\beta U(\cdot)]$, becomes also a functional of $n(\cdot)$. In ref. 3a (Theorem 9.1, p. 115) it has been shown that the condition

$$\int_{B(r, a/2)} n(z)\, dz \leqslant 1 \tag{52}$$

for any $r \in \Omega$ is a necessary condition for the inverse problem with hard-core potentials to have a solution. By taking $E = B(r, a/2) \equiv \{z \in \Omega: |z - r| \leqslant a/2\}$ and $\varepsilon = 1$ in (43), we see that (43), and thus (52), are satisfied with evolution of time when we choose the diameter a of the hard sphere small enough. Such adjustments of a are always possible as long as the bound (42) is independent of a. This is the case of Theorem 1. The case of the full revised Enskog equations hinges, among other things, on the convergence of the Mayer cluster series for g [see (6)]. As remarked earlier, relation (47) of Theorem 1 holds formally also for $i = \infty$, thus, in principle at least, making bound (42) independent of a. In the homogeneous case (n does not depend on r), the smallness of a is related to the smallness of $4/3\pi(a/2)^3\, n$, which is clearly less than one. Indeed, it is universally agreed (although not proved) that the close-packing density corresponds to $4/3\pi(a/2)^3\, n = \pi/\sqrt{18} \approx 0.74048$ (see, for example, ref. 21, p. 293). Thus, a stronger condition than (52) is required. We think that bound (38) might usefully serve as such a condition. Our motivation for this comes from ref. 3b, where the sufficient and necessary conditions to the inverse problem were given for a system in which some functionals of probability distributions were finite [see (3.6), p. 478 of ref. 3b]. In our case, we propose that bound (38) be the test for admissible models considered in the GET. We recall that (38) guarantees that Γ is bounded from below (in fact, bounded, in the case of the whole-space problem) and also implies (42).

5. A LOCAL VERSION OF $\Gamma(t)$ FOR THE GET

Another important property of the GET is that it has a local version of the Liapunov functional Γ. In the case of the RET such theorems have been proven in refs. 7 and 22. In ref. 23 such theorems have been obtained for various generalizations of the revised Enskog equation beyond the hard-core potential.

For a nonnegative solution of the generalized Enskog equation $f(t, r, v)$, we define a local Liapunov functional $\gamma(t, r)$ as follows:

$$n(t, r)\, \gamma(t, r) = \int_{R^3} f(t, r, v) \log f(t, r, v)\, dv - \int_0^t i(s)\, ds \tag{53}$$

where

$$i(t) = \tfrac{1}{2}a^2 \iiint_{R^3 \times R^3 \times S_+^2} [f(t, r - a\varepsilon, w)\, Y(t, r, v', r - a\varepsilon, w' \mid \Lambda f)$$
$$- f(t, r + a\varepsilon, w)\, Y(t, r, v, r + a\varepsilon, w \mid \Lambda f)]$$
$$\times f(t, r, v)\langle \varepsilon, v - w \rangle \, d\varepsilon \, dw \, dv \tag{54}$$

Proceeding in a similar way as in the proof of (15) and (3.8) of ref. 22, one obtains

$$\frac{\partial(n\gamma)}{\partial t} + \frac{\partial J^{\mathrm{GET}}}{\partial r} = \sigma^{\mathrm{GET}} \tag{55}$$

where

$$\sigma^{\mathrm{GET}} = -i(t) + \frac{1}{2} a^2 \iiint_{R^3 \times R^3 \times S_+^2} Y(t, r, v, r + a\varepsilon, w) \mid \Lambda f)$$
$$\times f(t, r, v)\, f(t, r + a\varepsilon, w)$$
$$\times \log \left[\frac{f(t, r, v')\, f(t, r + a\varepsilon, w')}{f(t, r, v)\, f(t, r + a\varepsilon, w)} \right] \langle \varepsilon, v - w \rangle \, d\varepsilon \, dw \, dv \tag{56}$$

and

$$J^{\mathrm{GET}} = \int_{R^3} [v - u(t, r)]\, f(t, r, v) \log f(t, r, v) \, dv$$
$$+ \frac{1}{2} a^3 \iiiint_{[0,1] \times R^3 \times R^3 \times S_+^2} Y(t, r - \lambda a\varepsilon, v, r + (1 - \lambda)\, a\varepsilon, w \mid \Lambda f)$$
$$\times f(t, r - \lambda a\varepsilon, v)\, f(t, r + (1 - \lambda)\, a\varepsilon, w)$$
$$\times \log \frac{f(t, r - \lambda a\varepsilon, v')}{f(t, r - \lambda a\varepsilon, v)} \langle \varepsilon, v - w \rangle \varepsilon \, d\varepsilon \, dw \, dv \, d\lambda \tag{57}$$

The change of the variables $(v, w) \rightleftharpoons (v', w')$ and $\varepsilon' = -\varepsilon$ in the first term of $i(t)$, together with the inequality $y(\log y - \log z) \geqslant y - z$ for $y > 0$ and $z > 0$, implies that

$$\sigma^{\mathrm{GET}} \leqslant 0 \tag{58}$$

When $\Gamma(t)$ can be considered as an H-function (see the discussion in Section 2), inequality (58) and Eq. (55) suggest that $s(t, r) \equiv -\gamma(t, r)$ can be viewed as a generalization of the entropy density for the GET with

$-\sigma^{\mathrm{GET}}$ as a nonnegative entropy production, and $-J^{\mathrm{GET}}$ linked to an entropy flux. We want to point out that only symmetry (8) of Y was used to derive Eq. (55) and inequality (58). We also observe that $-\sigma^{\mathrm{GET}}$ has the same functional form as in the RET, except, of course, for the much more general form of Y used in the GET. Now, for $Y = Y^{\mathrm{RET}}$, (55) reduces to the equation already derived in refs. 7 and 22, with the entropy production obtain in refs. 7 and 22 being equal to the $-\sigma^{\mathrm{GET}}$ of formula (56). Finally, integrating $n(t, r)\,\gamma(t, r)$ over $r \in \Omega$, we obtain $\Gamma(t)$, as defined in (13), together with inequality (16). Hence, Eq. (55) with inequality (58) is a local formulation of the Liapunov functional Γ.

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