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k-PARTICLE KINETIC EQUATIONS: IN SEARCH OF THE NONEQUILIBRIUM ENTROPY

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Systematic development of various Liapunov functionals (generalizations of the H–functions) in the kinetic theory is studied. The functionals are monotone functions of time, whose stationary points points determine the equilibria of the system governed by the corresponding kinetic equation. The mathematical structure is general enough to embrace kinetic equations for the N–particle distribution functions (the full hierarchy equations) as well as the kinetic equations of the reduced description, i.e., the equations for the k–particle distribution functions. In the case of the hierarchy of N equations (including the exact hierarchy) the stationary points of the functionals are of the same functional form as the k–particle distribution functions in the equilibrium statistical mechanics. For k=1 and the closure relation as in the revised Enskog equation, the first member of the family becomes the H–function found by Resibois [10]. As an application of the explicit form of the Liapunov functionals various existence and stability results for the corresponding kinetic equations are presented.

1. One-particle kinetic equations

Consider a gas composed of identical hard spheres of diameter

a, i.e., with the potential interaction given by

$$\phi^{HS}(r) = \begin{cases} \infty, & \text{for } r < a \\ 0, & \text{for } r \geq a. \end{cases} \tag{1.1}$$

When two particles of equal mass collide, their velocities v_1, v_2 take postcollisional values

$$v_1' = v_1 - \epsilon\langle\epsilon, v_1 - v_2\rangle, \qquad v_2' = v_2 + \epsilon\langle\epsilon, v_1 - v_2\rangle. \tag{1.2}$$

$\langle\cdot,\cdot\rangle$ 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. $\epsilon \in S_+^2 = \{\epsilon \in R^3 : |\epsilon| = 1, \langle v_1 - v_2, \epsilon\rangle \geq 0\}$.

Within the kinetic theory the state of fluid depends upon (among other things) the one–particle distribution function $f_1(t, r_1, v_1)$ representing at time t the number density of particles at point r_1 with velocity v_1. The exact rate of change of f_1 is given by

$$\frac{\partial f_1}{\partial t} + v_1 \frac{\partial f_1}{\partial r_1} = (N-1)a^2 \int dr_2 dv_2\, K_{12} f_2(t, r_1, v_1, r_2, v_2), \tag{1.3}$$

$$K_{12} f_2 = \int_{S_+^2} \left[\delta(r_{12} - a\epsilon) f_2' - \delta(r_{12} + a\epsilon) f_2\right] \langle\epsilon, v_1 - v_2\rangle\, d\epsilon,$$

with $r_{12} = r_1 - r_2$, and velocities in f_2' computed according (1.2). The density of pairs of particles in collisional configurations is described by the two-particle distribution function f_2. The above equation is the first of the infinity BBGKY–hierarchy for hard spheres.

In order for equation (1.3) to be operational one needs a closure relation for f_2. As usual, one defines the two-particle correlation function Y by the following relation:

$$f_2(t, r_1, v_1, r_2, v_2) = Y\, f_1(t, r_1, v_1)\, f_1(t, r_2, v_2). \tag{1.4}$$

Various choices of Y define different kinetic equations known in the literature. For $Y \equiv 1$ (i.e., no velocity and configurational correlations) and $a = 0$ one obtains the classical Boltzamnn equation. If $f_1 \geq 0$ is a solution of the Boltzmann equation then

$$H_B(t) = \int\int f_1(t, r_1, v_1) \log f_1(t, r_1, v_1)\, dv_1 dr_1 \tag{1.5}$$

is such that (the H–theorem) $dH_B/dt \le 0$, with equality only when f_1 is a local Maxwellian.

In the revised Enskog equation $Y = Y^{REE}$ [1], where Y^{REE} is the pair correlation function for a system, in which, at any time, the only correlations are due to the excluded volume of the spheres. In particular, there are no correlations between velocities in the system. Y^{REE} can be written explicitly in terms of the Mayer cluster expansion (see [11], [9], and [2]).

For nonnegative solutions, f_1, of the revised Enskog equation I define (see [10], [7], and [8])

$$H_{REE}(t) = \int f_1 \log f_1 \, dv_1 dr_1 - (N-1)a^2 \int_0^t I(s)\, ds, \tag{1.6}$$

where

$$2I(t) = \int d\epsilon dv_2 dv_1 dr_1 \Big[f_1(t, r_1 - a\epsilon, v_2) Y^{REE}(r_1, r_1 - a\epsilon)$$
$$- f_1(t, r_1 + a\epsilon, v_2) Y^{REE}(r_1, r_1 + a\epsilon) \Big] f_1(t, r_1, v_1) \langle \epsilon, v_1 - v_2 \rangle.$$

$H_{REE}(t)$ has the property

$$\frac{dH_{REE}}{dt} \le 0. \tag{1.7}$$

The functional H_{REE} has the form $H_B(t) + H_{corr}(t)$. Furthermore, one can express $H_{corr}(t)$ explicitly in terms of the Mayer graphs (see [5], [9], and [2])

$$H_{corr}(t) = (N-1) \sum_{k=2}^{\infty} \frac{1}{k!} \int dr_1 \cdots \int dr_k \, n(2) \ldots n(k)\, V(1 \ldots k),$$

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

In contrast to Botzmann's H–function, $H_{REE}(t)$ consists of two parts: the kinetic part ($H_B(t)$) and the correlational part. $H_{REE}(t)$ (modulo an additive constant) has a functional form of the equilibrium (non–uniform) entropy for the infinity system of hard spheres.

The same functional form (see (1.6)) of the Liapunov functional is retained for Y having the following form (see [8] and [9]):

$$Y \equiv Y(t,\, r_1,\, v_1,\, r_2,\, v_2\,|\,\Lambda f_1(t)). \tag{1.8}$$

Form (1.8) also includes Y equal to the exact two–particle correlation function.

Here, for each fixed $t \geq 0$, Λ indicates an operator, possibly nonlinear, acting on f_1, and $|\,\Lambda f_1(t)$ denotes the functional dependence of Y on $\Lambda f_1(t)$ (typically Λ represents moments of f_1; in the case of the revised Enskog equation Λ represents the zeroth moment of f_1). The principal assumption is that Λ and $|\,\Lambda f_1(t)$ act in such a way that Y is symmetric under the exchange of variables $r_1, v_1 \rightleftharpoons r_2, v_2$, and that Y is nonegative for $f_1 \geq 0$.

I end this section with the theorem that utilizes the form of the Liapunov functional in (1.6).

EXISTENCE THEOREM ([9], [2]) *Suppose that $T > 0$, Y is regular, and $f_0 \geq 0$ satisfies*

$$\int\!\!\int (1 + v_1^2 + r_1^2 + |\log f_0|) f_0 \, dv_1 dr_1 = C_0 < \infty. \tag{1.9}$$

In addition, assume that there exists $C_{corr}(T) > 0$ such that

$$H_{corr}(t) \geq C_{corr} > -\infty, \tag{1.10}$$

uniformly in $t \in [0,T]$. Then there exists a mild solution $f_1(t, r_1, v_1)$ such that $\lim_{t\to 0^+} f_1(t, r_1, v_1) = f_0(r_1, v_1)$ *a.e. in* (r_1, v_1).

2. The main construction for the hierarchy equations

For classical systems in equilibrium the entropy is defined by

$$S_{fine} = -\int \cdots \int P_N \log P_N \, d(1) \cdots d(i) \cdots d(N), \tag{2.1}$$

where $(i) \equiv (r_i, v_i)$ and P_N is the symmetric N–particle probability density (N denotes the number of particles in the system).

The use of the fine–grained entropy S_{fine} is not adequate in the above nonequilibrium situation. Indeed, by the Liouville theorem (volume element in the phase space is invariant under time evolution), one has

$$\frac{d}{dt}S_{fine} = 0, \quad \text{for all} \quad t \geq 0. \tag{2.2}$$

In other words, the fine–grained entropy becomes trivial in the above nonequilibrium situation. I recall that in equilibrium the form of S_{fine} was determined by two factors: (1) that an adiabatic process cannot decrease the entropy, and (2) that the entropies of independent systems are additive.

There are no generally accepted rules for defining the nonequilibrium entropy. However, by analogy with equilibrium (see, for example, [6]), one would like the entropy to satisfy similar conditions, in particular, that of non–decrease, and also to be equal to the equilibrium entropy when the ensemble is in equilibrium.

Finally, the concept of the nonequilibrium entropy has been also influenced by the information's theory negative entropy, which measures loss of the information about the system with time evolution. As I will show below, an analog of this, applied to the concept of the reduced description given by the k–particle distribution function $P_N^{(k)} = \int P_N d(k+1)\cdots d(N)$, for $1 \leq k < N$, is very revealing.

The Liouville equation can be transformed into equivalent system of N equation for $P_N^{(k)}$. Integration with respect to the positions and velocities (r_i, v_i) of $N-k$ particles, for $k = 1, \ldots, N$ and using the laws of elastic collisions yields

$$\begin{aligned} &\frac{\partial P_N^{(k)}}{\partial t} + \sum_{i=1}^{k} v_i \frac{\partial P_N^{(k)}}{\partial r_i} = E_k(P_N^{(k+1)}) \equiv \\ &(N-k)a^2 \sum_{i=1}^{k} \int_{R^3 \times S^2_{i,+}} \int \left[P_N^{(i+1)\prime} - P_N^{(i+1)} \right] \langle v_i - w, \epsilon \rangle \, d\epsilon dw, \end{aligned} \tag{2.3}$$

where $S^2_{i,+} = \{\epsilon : |\epsilon| = 1, \langle \epsilon, v_i - w \rangle \geq 0\}$ and velocities in $P_N^{(k+1)\prime}$ are computed according to the hard–spheres collision laws. Equations (2.3) represent the exact system (BBGKY–hierarchy) of N–particle hard–sphere kinetic equations.

Next, I want to indicate that system (2.3) admits an analog of the collision invariants and an H–function.

Collision invariants

For $k \geq 1$, $\psi(1,\ldots,k)$ measurable and $P_N^{(k)} \in \acute{C}_0$ one has

$$\int E_k(P_N^{(k+1)})\psi(1,\ldots,k)\, d(1)\cdots d(k) = 0 \tag{2.4}$$

for all $\psi(1,\ldots,k)$ of the form

$$\psi(1,\ldots,k) = \prod_{i=1}^{k} \left[h_i(r_1,\ldots,r_k) + \langle C_{i1}, v_i\rangle + C_{i2}v_i^2\right], \tag{2.5}$$

where, for $i = 1,\ldots,k$, h_i are arbitrary measurable functions, C_{i1} are constant vectors and C_{i2} are scalar constants. ψ are generalizations of Boltzmann's collison invariants.

The Liapunov functionals – An analog of the H–theorem

For nonnegative solutions $P_N^{(k)}$ of (2.3) and for $1 \leq k \leq N$, I consider

$$\Gamma_k(t) = \int P_N^{(k)} \log P_N^{(k)}\, d(1)\cdots d(k) + \sum_{i=1}^{k}\int_0^t I_i^k(s)\, ds. \tag{2.6}$$

The functions $I_i^k(t)$ are defined by

$$I_i^k(t) = -\frac{(N-k)a^2}{2}\int d\epsilon dw d(1)\cdots d(k)\langle\epsilon, v_i - w\rangle G^k \times \tag{2.7}$$

$$\left[P_N^{(k)}(r_i, v_i')P_N^{(k)}(r_i + a\epsilon, w') - -P_N^{(k)}(r_i, v_i)P_N^{(k)}(r_i + a\epsilon, w)\right],$$

where the functions G^k depend only on $P_N^{(k)}$. For $\Gamma_k(t)$ as given above, one obtains, for $1 \leq k \leq N$,

$$\frac{d\Gamma_k}{dt} \leq 0. \tag{2.8}$$

For $k = N$ $\Gamma_N(t)$ becomes the fine–grained entropy S_{fine}.

In addition, one can completely describe all solutions for which $d\Gamma_k(t)/dt = 0$. This is done under already assumed symmetry of P_N, which also implies the symmetry of $P_N^{(k)}$, for $1 \le k \le N-1$. One can show that $d\Gamma_k(t)/dt = 0$ if and only if

(2.9)
$$P_N^{(k)} = \alpha_k(t, r_1, \ldots, r_k)\big(\beta_k(t)m/2\pi\big)^{3/2} \prod_{i=1}^{k} \exp\left(-\beta_k(t)m\big(v_i - u_k(t)\big)^2/2\right),$$

where $\alpha_k(t, r_1 \ldots, r_k)$ is an arbitrary and symmetric function of its arguments. In equilibrium, except for a multiplicative constant, α_k becomes the k–particle correlation function. Here, $\beta_k(t)$ and $u_k(t)$ for $k = 1, \ldots, N-1$ are arbitrary measurable functions of t.

Inequalities (2.8) reflect the fact that the information about the system available to us in the description on the k–particle level $(k < N)$ is greatly reduced as compared to the complete information about the system on the N–particle level.

3. Special cases.

In the case of $k = 1$, and the closure relation as in the revised Enskog theory, $\Gamma_1(t)$ becomes the H–function found by Resibois [10]. Recently, jointly with G. Stell [9], we considered a class of hard–sphere kinetic equations (on 1–particle level), called the generalized Enskog equation (GEE), that follows from the first BBGKY–hierarchy equation and the closure relation for $P_N^{(2)}$

(3.1)
$$P_N^{(2)}(t, 1, 2) = G(t, 1, 2)P_N^{(1)}(t, 1)P_N^{(1)}(t, 2).$$

The Liapunov functional obtained there is precisely $\Gamma_1(t)$, where it plays a fundamental role in existence theorems.

In the case of Grad's limit, $\Gamma_1(t)$ reduces to Boltzmann's H–function. In fact, in this case $I_1^1(t) \equiv 0$.

Another interesting case in which all $I_i^k(t) \equiv 0$ is provided in the limit $N \to \infty$, $a \to 0$, with Na^2 bounded, and for solutions in the factorized form (see [3], pp. 53-54]). In the just describe case the

Liapunov functionals $\Gamma_k(t)$ $(1 \leq k < \infty)$ reduce to

$$\Gamma_k(t) = \int P^{(k)} \log P^{(k)}\, d(1) \cdots d(k), \tag{3.2}$$

where $P^{(k)} = \lim_{N\to\infty} P_N^{(k)}$, in some sense to be specified. This result fully agrees with Grad's observation [4] that, for symmetric functions $P^{(k)}$, the informational entropy gives the correct minimum only for $P^{(k)}$ in the factorized form, in which case, it is really Boltzmann's H–function that covers the situation.

For simplicity, I have considered here only one–component gas of hard–spheres. The results can be extended to multicomponent and chemically reacting fluids.

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