

H-Theorem for an Infinite, One-Dimensional, Hard-Point System

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Received January 8, 1980

We use a well-studied soluble model to define a nonequilibrium entropy. This entropy has all the required properties; in particular, it is not time-reversal invariant, so that its monotonic increase in time also shows up after we perform a velocity inversion "experiment."

KEY WORDS: Exactly soluble model; irreversible phenomena; *H*-theorem; velocity inversion.

1. INTRODUCTION

Exactly soluble models have been extensively used in statistical mechanics. Very often they provide a way of testing the approximations that are introduced in more general theories. In the case of the problem of approach to equilibrium, they have served as guides for understanding how one can obtain an irreversible macroscopic description starting from the dynamical equations of motion. Of course one cannot expect a general solution to this long-standing problem simply by looking at these models, which are, in general, very pathological. However, the existence of at least one infinite dynamical system where the irreversible description is exact is important by itself. Besides, such models are also pedagogical in the sense that the physical processes taking place are easier to study.

The model we study in this paper has already been investigated from this point of view in Ref. 1. It has a very peculiar property: provided no

Supported financially by the Belgian Government, Actions de Recherches Concertées, Convention 76/81, II.3.

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initial correlations exist among the particles, then the Boltzmann equation gives the exact description of the evolution of the one-particle distribution function. This property makes the model interesting for a study of the relation between the kinetic equations and the underlying reversible dynamics. In Ref. 1 we analyzed this relation by solving explicitly the Loschmidt paradox in this model. Here we want to construct a functional which has all the desired properties for a nonequilibrium entropy.⁽⁴⁾

The system is an assembly of N hard points moving on a line of length L and we shall be interested in the time evolution of the reduced distribution functions in the so-called thermodynamic limit, i.e., letting $L \rightarrow \infty$, $N \rightarrow \infty$, with $N/L = \rho$ remaining finite. We shall limit ourselves to the particular case of a local perturbation of equilibrium, so that the equations will be linear. From a mathematically rigorous point of view, it has been shown that, given such initial conditions, the hierarchy (BBGKY) equations for the infinite system have a unique solution in the space of sequences of bounded functions.⁽¹²⁾ Also, the ergodic properties of the infinite system of hard rods has been studied,⁽⁶⁾ and that system is known to be a Bernoulli flow, whereas the finite system is not even ergodic. However, the relation of these ergodic properties to the kinetic description is still an open question. For instance, the Bernoulli flow property is sufficient for the existence of an H -theorem⁽⁷⁾; however, it does not imply the correctness of an irreversible kinetic equation, or, even more, the existence of a transport coefficient.

These kinetic properties have been extensively studied in our model.^(2,5,8) One knows exactly the self-diffusion coefficient⁽⁵⁾ and this has allowed a study of the nonanalytic density expansion. As already mentioned, when the velocities of the rods take discrete values the collision operator of the kinetic equation for the one-particle distribution function has a purely discrete spectrum; it reduces to the Boltzmann collision operator. In Ref. 1 we generalized this kinetic equation by taking into account the effect of the initial correlations, which are, of course, essential in the case of velocity inversion. In this paper we want to show that there is a similar kinetic description of the correlations—more precisely, the nonfactorizable parts of the n -particle distribution functions—and use this description to define a nonequilibrium entropy. This construction will be based on a very peculiar property of the model with two allowed velocities, namely that the reduced phase space can be split into two orthogonal subspaces, a precollisional and a postcollisional part, and there is an irreversible flow from the first part to the other.

We shall proceed as follows. We first recall the properties of the model and its “Liouville” equation of motion, and define the reduced quantities, which we assume remain finite in the thermodynamic limit.

The next section is devoted to the derivation of the kinetic equations. Because the methods have already been given in a preceding article and the calculations involved are not difficult but tedious, we simply state most of the results. The main property which will be needed is the existence of two orthogonal projections such that reduced distribution functions will be split in two parts, one of which will evolve independent of its complement. Although there cannot be an H -theorem for the entire set of reduced functions, we shall define an H -function which depends on the projections of the reduced functions and which has a monotonic decrease in time.

In the last section we finally illustrate this irreversible behavior by calculating the entropy before and after a velocity inversion has been performed; indeed, with our definition, the entropy has a jump during the velocity inversion so that, after it, it increases again monotonically. Most of the results are given without detailed proofs; these will be published elsewhere.⁽¹⁴⁾

2. THE MODEL AND ITS PROPERTIES

The model we shall study is a simplification of the one-dimensional, infinite, hard-rod system. First of all the system is supposed to be at equilibrium except for the statistical properties of a tagged particle located near the origin and having correlations of finite range with its neighbors. Under these conditions, the dynamical evolution is similar to that of a Rayleigh model where only the labeled particle interacts with otherwise freely moving bath particles.⁽⁸⁾ Moreover, we suppose the system is made up of points having two allowed velocities; the first simplification has no important consequences, as it is known that thermodynamic properties of hard rods of length d are recovered by substituting $\rho \rightarrow \rho(1 - \rho d)^{-1}$ in the results for points.⁽⁸⁾ The second simplification is more drastic, in that it is responsible for a purely point spectrum of the collision operator, leading therefore to a pure exponential decay for the velocity autocorrelation function. However, the point is that, as such, the model is still of a dynamical nature.

The usual approach for the study of nonequilibrium properties has to be modified because of the singular nature of the interaction potential. In particular, a limiting procedure is required in order to define a so-called "pseudo-Liouville" operator.^(9,10)

Let $\rho_N(r_1, c_1, \{r_i, c_i\}; t)$, $i = 2, \dots, N$, be the N -particle distribution function of the system at time t : it is a positive, bounded, normalized function and symmetric with respect to the interchange of two bath particles. Its equation of motion reads

$$i \partial \rho_N / \partial t = L_N \rho_N \quad (2.1)$$

We refer to Equation (2.1) as to the pseudo-Liouville equation because of the singular character of the L_N operator. In our case the L_N operator can be written^(1,9)

$$L_N = L_N^0 + \delta L_n \quad (2.2)$$

$$L_N^0 = -i \sum_{a=1}^N c_a \frac{\partial}{\partial r_a} \quad (2.3)$$

$$\delta L_n = i \sum_{a=2}^N K_{1a} \quad (2.4)$$

$$K_{1a} = (2c) \delta(r_1 - r_a) [P_{1a} - 1] d\eta_{1a} \quad (2.5)$$

where

$$c_a = \pm c \quad (2.6)$$

$$P_{1a} f(c_1, c_a) = f(c_a, c_1) \quad (2.7)$$

$$d\eta_{1a} f(r_1, r_a) = f(r_1 - \eta c_1, r_a - \eta c_a); \quad \eta > 0 \quad (2.8)$$

$d\eta_{1a}$ is an infinitesimal displacement operator; η is a small, positive quantity, set to zero at the end of the calculations. It is necessary because K_{1a} is singular at $r_1 = r_a$ and it acts on discontinuous functions at this point. Indeed $\rho_N(t)$ is a continuous function along the trajectories in phase space: however, these trajectories are discontinuous because collisions are instantaneous. The displacement operator therefore determines if one has to take $\rho_N(t)$ before or after the collision at $r_1 = r_a$. With such a rule, one can show that a suitably chosen "norm" $\int \rho_N^2(t) dx^N \cdot dv^N$ for a system of hard spheres is constant in time, as it should be.⁽³⁾ An alternative way of writing Eq. (2.5) is

$$K_{1a} = (2c) [\delta(r_1 - r_a - (c_1 - c_a)\eta) P_{1a} - \delta(r_1 - r_a + (c_1 - c_a)\eta)] \quad (2.9)$$

so that the singularity of K_{1a} is at the left or the right of the jump of $\rho_N(t)$ at $r_1 = r_a$.

An important property linked with the operator K_{1a} is that there exists in the infinite two-particle phase space a projector $P_a = P_a^2$ such that

$$K_{1a} = (1 - P_a) K_{1a} P_a \quad (2.10)$$

The explicit expression for P_a is [$\eta(x)$ is the Heaviside function]

$$P_a = \eta(r_1 - r_a) \delta_{c_a, +c}^{Kr} + \eta(-r_1 + r_a) \delta_{c_a, -c}^{Kr} \quad (2.11)$$

Equation (2.10) means that there is a partition of the pair phase space such that K_{1a} acts on only one part, namely the P_a subspace. Points in the complementary subspace will not be able to go to the P_a part; recollisions are impossible for the infinite system (indeed, in Ref. 1 they have been shown to give contributions of order $1/L$). We can reformulate the main

lemma stated in Ref. 1 with the help of this projection. Let us define $L_{(N-a)}$ by

$$L_N = L_{(N-a)} + iK_{1a} \tag{2.12}$$

Then it is readily shown that

$$P_a \{ \exp[-iL_{(N-a)}t] \} (1 - P_a) = 0 \tag{2.13}$$

so that it implies

$$K_{1a} \{ \exp[-iL_{(N-a)}t] \} K_{1a} = 0 \tag{2.14}$$

which is Eq. (2.15) of Ref. 1. Of course such a property is only true after having taken the thermodynamic limit.

Let us also mention another difficulty due to the discontinuous nature of $\rho_N(t)$ at the point of contact of two rods. $\rho_N(t)$ should vanish for overlapping configurations. However, one may continue $\rho_N(t)$ inside overlapping configurations so it can be derived, and then multiply it by a weight function which is 1 everywhere except for overlapping configurations, where it vanishes. Such a procedure is impossible for points. However, we can follow the procedure for rods of nonzero diameter d and then take the limit $d \rightarrow 0$.

Let $f(r)$ and $g(r)$ be two continuous and square summable functions except for a discontinuity at $r = 0$. Then we give the following meaning to the expression

$$\begin{aligned} & \int_{-\infty}^{+\infty} dr f(r) \frac{\partial g(r)}{\partial r} \\ &= \lim_{d \rightarrow 0} \left\{ \int_{-\infty}^{+\infty} dr W(r-d) f(r) \frac{\partial g(r)}{\partial r} \right. \\ & \quad \left. + \int dr f(r) g(r) [\delta(r-d) - \delta(r+d)] \right\} \end{aligned} \tag{2.15}$$

where

$$\begin{aligned} W(r-d) &= 0, & |r| \leq d \\ &= 1, & r > d \end{aligned} \tag{2.16}$$

so that

$$\begin{aligned} & \int dr f(r) \frac{\partial g(r)}{\partial r} \\ &= \lim_{d \rightarrow 0} \left[\left\{ \int_{-\infty}^{+d} + \int_{+d}^{+\infty} \right\} f(r) \frac{\partial g(r)}{\partial r} \right. \\ & \quad \left. + f(+d)g(+d) - g(-d)f(-d) \right] \end{aligned} \tag{2.17}$$

The interpretation given in Eq. (2.17) may be shown to be consistent with conservation properties along the free motion trajectories.

3. KINETIC EQUATIONS

3.1. Reduced Distribution Functions

Let us briefly recall the definitions of the well-behaved functions at the thermodynamic limit. The formalism we use has been developed in Ref. 11 for the study of dense fluids.

We start with the expansion of $\rho_N(t)$ in clusters:

$$\rho_N(t) = \sum_{l=1}^N \sum_{\{l\}} \delta\rho_{N,l}(r_1, \{r_l\}, c_1, \dots, c_N; t) \quad (3.1)$$

where $\{l\}$ is a set of l particles, $1, i_1, \dots, i_{l-1} \in 1, \dots, N$. Introducing the one-particle projector

$$P_i = \frac{1}{L} \int_{-L/2}^{+L/2} dr_i \dots \quad (3.2)$$

and its complement $Q_i = 1 - P_i$, we obtain that $\delta\rho_{N,l}(t)$ is given by

$$\delta\rho_{N,l}(t) = \left(\prod_{j \notin \{l\}} P_j \right) \left(\prod_{i \in \{l\}} Q_i \right) \rho_N(t) \quad (3.3)$$

Since the system is finite, we have to define boundary conditions, which we take periodic; however, since the size of the system L goes to infinity together with N , but $N/L = \rho$ remains finite, these periodic conditions have no influence. We denote this limit by \lim_{∞} . We make the hypothesis that the following quantity is well behaved in the thermodynamic limit:

$$\begin{aligned} & \delta\varphi_{n,l}(r_1, \dots, r_l, c_1, \dots, c_n; t) \\ &= \lim_{\infty} L^{N-1} \sum_{c_{n+1}, \dots, c_N} \delta\rho_{N,l}(r_1, \{r_l\}, c_1, \dots, c_N; t) \end{aligned} \quad (3.4)$$

Moreover, we impose that at $t = 0$

$$\begin{aligned} & \delta\varphi_{n,l}(r_1, \dots, r_l, c_1, \dots, c_n; 0) \\ &= \left(\frac{1}{2}\right)^{n-l} \delta\varphi_{l,l}(r_1, \dots, r_l, c_1, \dots, c_l; 0), \quad n \geq l \end{aligned} \quad (3.5)$$

$$\delta\varphi_{l,l}(0) \Big|_{|r_1 - r_l| \rightarrow \infty} \rightarrow 0, \quad i \in \{l\} \quad (3.6)$$

These two relations express the fact that there is no long-range correlation

at $t = 0$. The n -particle distribution function is defined, as usual, as

$$f_n(r_1, \dots, r_n, c_1, \dots, c_n; t) = \lim_{\infty} \frac{(N-1)!}{(N-n)!} \int dr_{n+1} \dots dr_N \sum_{c_{n+1}, \dots, c_N} \rho_N(t) \quad (3.7)$$

We introduce a function which we call the n -particle correlation $\delta f_n(t)$ ($\delta f_1 \equiv f_1!$),

$$\delta f_n(r_1, \dots, r_n, c_1, \dots, c_n; t) = \rho^n \delta \varphi_{n,n}(r_1, \dots, r_n, c_1, \dots, c_n; t) \quad (3.8)$$

and obtain the most general form of initial conditions in terms of reduced functions:

$$f_n(r_1, \dots, r_n, c_1, \dots, c_n; 0) = \left(\frac{\rho}{2}\right)^{n-1} f(r_1, c_1, 0) + \left(\frac{\rho}{2}\right)^{n-2} \sum_{a=2}^n \delta f_2(r_1, r_a, c_1, c_a; 0) + \dots + \delta f_n(r_1, \dots, r_n, c_1, \dots, c_n; 0) \quad (3.9)$$

In Ref. 1 we have shown that the decomposition (3.9), or equivalently the properties (3.6) and (3.7), propagate in time. Correlations between the tagged particle and bath particles are created during the evolution, but they are localized in space so that Eq. (3.9) is still meaningful.

3.2. Reduced Equations

The equations obeyed by $f_1(t), \delta f_2(t), \dots$ are derived as follows: first we write the master equation for the projection of $\rho_N(t)$:

$$P_N = \prod_{i=2}^N P_i \quad (3.10)$$

$$\frac{\partial P_N \rho_N(t)}{\partial t} = \int_0^t G_N(\tau) P_N \rho_N(t-\tau) + \mathcal{D}_N(Q_N \rho_N(0); t) \quad (3.11)$$

$$Q_N \rho_N(t) = \int_0^t C_N(\tau) P_N \rho_N(t-\tau) + \mathcal{P}_N(Q_N \rho_N(0); t) \quad (3.12)$$

We then multiply each equation by L^{N-1} , sum over the velocities, and take the thermodynamic limit—see the definitions (3.4) and (3.8). Calculations are long and tedious, but without any surprises; they amount to showing that terms involving recollisions of the tagged particle with any other bath particle are indeed of order $1/L$ and thus strictly zero in the thermodynamic limit. Besides, one gets a Boltzmann propagator for the tagged

particle, or, equivalently, the equation of motion for $f_1(r_1, c_1, t)$ reads

$$\frac{\partial f_1}{\partial t} = \left(-c_1 \frac{\partial}{\partial r_1} + \mathbf{C} \right) f_1(r_1, c_1, t) + \mathfrak{D}_1(r_1, c_1; t) \quad (3.13)$$

where

$$\mathbf{C}f_1(r_1, c_1, t) = (\rho c) [f_1(r_1, -c_1, t) - f_1(r_1, c_1, t)] \quad (3.14)$$

and the so-called destruction term is given by

$$\mathfrak{D}_1(r_1, c_1; t) = \sum_{n=2}^{\infty} \mathfrak{D}_1^{(n)}(\delta f_n(0); t) \quad (3.15)$$

$$\begin{aligned} & \mathfrak{D}_1^{(n)}(\delta f_n(0); t) \\ &= \int_0^t dt_1 \cdots \int_0^{t_{n-3}} dt_{n-2} \int dr_2 \cdots dr_n \sum_{c_2 \cdots c_n} K_{12} \\ & \times \exp \left[(t - t_1) \left(-c_1 \frac{\partial}{\partial r_1} - c_2 \frac{\partial}{\partial r_2} + \mathbf{C} \right) \right] K_{13} \\ & \times \cdots \exp \left[(t_{n-2} - 0) \left(-c_1 \frac{\partial}{\partial r_1} \cdots - c_n \frac{\partial}{\partial r_n} + \mathbf{C} \right) \right] \delta f_n(0) \end{aligned} \quad (3.16)$$

We can give a simple physical meaning for this expression: an n -particle correlation influences the evolution of f_1 after these n particles have all collided with the tagged particle. Between collisions one has a damped propagator. A graphical representation has been introduced in Ref. 1 to sketch such events.

When no correlations are present at $t = 0$, Eq. (3.13) reduces to the Boltzmann equation.^(2,5) It should be noted that correlations will be created as time increases. However, the correlations created do not influence the evolution of f_1 ; indeed they are in the postcollisional subspace, which is well separated from the precollisional subspace—see Eq. (3.14). This is the reason why the collision operator \mathbf{C} is strictly Markovian, and so there is no arbitrariness in choosing the initial time.

The preceding argument suggests that the part of the correlations that are in the precollisional subspace obey a separate equation of motion. This is even more obvious if we compare Eq. (3.13), together with (3.16), with the corresponding hierarchy equation as derived, for example, in Ref. 11; this last equation reads

$$\frac{\partial f_1}{\partial t} = \left(-c_1 \frac{\partial}{\partial r_1} + \mathbf{C} \right) f_1 + \int dx_2 \sum_{c_2} K_{12} \delta f_2(t) \quad (3.17)$$

This implies that the part of $\delta f_2(t)$ that influences $f_1(t)$ depends on $\{\delta f_n(0)\}$, $n \geq 2$; moreover, that part of $\delta f_2(t)$ belongs to the P_2 subspace [see Eq. (2.11)].

To be more precise, let us define the precollisional correlation

$$\Delta f_2(t) = (2/\rho)P_2 \delta f_2(t) \quad (3.18)$$

and its complement

$$\widehat{\Delta f_2}(t) = (1 - P_2) \delta f_2(t) \quad (3.19)$$

More generally, for any n

$$\Delta f_n(t) = (2/\rho)^{n-1} (P_1 \dots P_n) \delta f_n(t) \quad (3.20)$$

and

$$\widehat{\Delta f_n}(t) = \delta f_n(t) - (\rho/2)^{n-1} \Delta f_n(t) \quad (3.21)$$

Then we should be able to prove that there is a separate equation for the evolution of $\Delta f_n(t)$, which depends only on $\Delta f_n(t)$ and $\Delta f_{m \geq n}(0)$, and another for $\widehat{\Delta f_n}(t)$, which could be a functional of $\Delta f_n(t)$. This is indeed the case.

We start from the master equation, Eq. (3.12), multiply it by L^{N-1} , sum over the velocities c_3, \dots, c_N , integrate over space variables, and take the thermodynamic limit; one gets for $\delta f_2(t)$

$$\begin{aligned} \delta f_2(t) = & \left(\frac{2}{\rho} \right) \int_0^t dt_1 \exp \left[\left(-c_1 \frac{\partial}{\partial r_1} - c_2 \frac{\partial}{\partial r_2} + C \right) (t - t_1) \right] K_{12} f_1(t_1) \\ & + \exp \left[\left(-c_1 \frac{\partial}{\partial r_1} - c_2 \frac{\partial}{\partial r_2} + C \right) t \right] \delta f_2(0) \\ & + \int_0^t dt_1 \exp \left[\left(-c_1 \frac{\partial}{\partial r_1} - c_2 \frac{\partial}{\partial r_2} + C \right) (t - t_1) \right] K_{12} \\ & \times \exp \left[\left(-c_1 \frac{\partial}{\partial r_1} - c_2 \frac{\partial}{\partial r_2} + C \right) t_1 \right] \delta f_2(0) \\ & + \frac{\rho}{2} \int dr_3 \sum_{c_3} \int_0^t dt_1 \int_0^{t_1} dt_2 \exp \left[\left(-c_1 \frac{\partial}{\partial r_1} - c_2 \frac{\partial}{\partial r_2} + C \right) (t - t_1) \right] \\ & \times K_{13} \exp \left[\left(-c_1 \frac{\partial}{\partial r_1} - c_2 \frac{\partial}{\partial r_2} - c_3 \frac{\partial}{\partial r_3} + C \right) (t_1 - t_2) \right] \\ & \times K_{12} \exp \left[\left(-c_1 \frac{\partial}{\partial r_1} - c_3 \frac{\partial}{\partial r_3} + C \right) t_2 \right] \delta f_2(c_1, c_3, r_1, r_3; 0) \\ & + \int_0^t dt_1 \exp \left[\left(-c_1 \frac{\partial}{\partial r_1} - c_2 \frac{\partial}{\partial r_2} + C \right) (t - t_1) \right] \mathcal{Q}_2(t_1) \end{aligned} \quad (3.22)$$

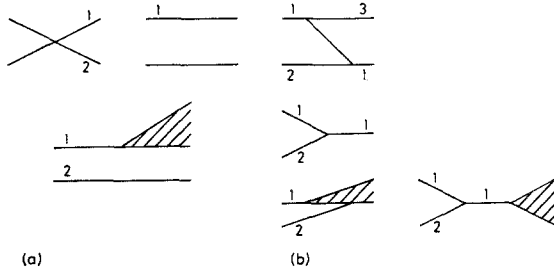


Fig. 1. (a) Graphs contributing to $\Delta f_2(t)$ only; (b) those contributing to $\delta f_2(t)$ and not to $\Delta f_2(t)$.

In Eq. (3.22) we have grouped all contributions coming from $\delta f_{n \geq 3}(0)$ in the destruction term $\mathcal{D}_2(t_1)$. All the terms contributing to $\delta f_2(t)$ may be represented by graphs. This is shown in Fig. 1, where we distinguish between graphs contributing to $\delta f_2(t)$ and those contributing to $\Delta f_2(t)$. The analytic expression for $\Delta f_2(t)$ is simple:

$$\Delta f_2(t) = \exp\left[\left(-c_1 \frac{\partial}{\partial r_1} - c_2 \frac{\partial}{\partial r_2} + C\right)t\right] \frac{2}{\rho} \delta f_2(0) + \frac{2}{\rho} \int_0^t dt_1 \exp\left[\left(-c_1 \frac{\partial}{\partial r_1} - c_2 \frac{\partial}{\partial r_2} + C\right)(t - t_1)\right] \bar{D}_2(t_1) \quad (3.23)$$

and $\bar{D}_2(t_1)$ is the part of $\mathcal{D}_2(t_1)$ that has no K_{12} interaction (see Fig. 1). Now the remarkable feature of Eq. (3.23) is that it has the same form as the solution $f_1(r_1, c_1, t)$ and therefore the equation of motion for $\Delta f_2(t)$ must be similar to Eq. (3.13). This is indeed so if we restrict the space to the P_2 subspace; taking the derivative of Eq. (3.23), one gets

$$\frac{\partial \Delta f_2(t)}{\partial t} = \left(-c_1 \frac{\partial}{\partial r_1} - c_2 \frac{\partial}{\partial r_2} + C\right) \Delta f_2(t) + \bar{D}_2(t) \quad (3.24)$$

where

$$\bar{D}_2(t) = \sum_{n=3}^{\infty} \bar{D}_2^{(n)}(\Delta f_n(0) | t) \quad (3.25)$$

$$\begin{aligned} &\bar{D}_2^{(n)}(\Delta f_n(0) | t) \\ &= \int dr_3 \cdots dr_n \sum_{c_3 \cdots c_n} \int_0^t dt_1 \cdots \int_0^{t_{n-4}} dt_{n-3} \\ &\times K_{13} \exp\left[\left(-c_1 \frac{\partial}{\partial r_1} - c_2 \frac{\partial}{\partial r_2} - c_3 \frac{\partial}{\partial r_3} + C\right)(t - t_1)\right] K_{14} \\ &\times \cdots K_{1n} \exp\left[\left(-c_1 \frac{\partial}{\partial r_1} \cdots - c_n \frac{\partial}{\partial r_n} + C\right)t_{n-3}\right] \left(\frac{\rho}{2}\right)^n \Delta f_n(0) \end{aligned} \quad (3.26)$$

Equation (3.24) could be made valid in the entire pair space by the addition of a singular operator, similar to the collision operator K_{12} ; however, as we shall not need this continuation, we shall use Eq. (3.24) and restrict its validity to the P_2 subspace. The generalization to higher order correlations $\Delta f_n(t)$ is straightforward,

$$\frac{\partial \Delta f_n(t)}{\partial t} = \left(-c_1 \frac{\partial}{\partial r_1} \cdots - c_n \frac{\partial}{\partial r_n} + C \right) \Delta f_n(t) + \bar{D}_n(t) \quad (3.27)$$

where the expression for $\bar{D}_n(t)$ is an obvious generalization of Eq. (3.26).

Finally, this set of equations can be written in a simple form, which we shall use in the next section. Introducing the dimensionless variables

$$\begin{aligned} \tau &= t(1/\rho c) \\ x_i &= r_i \rho \\ v_i &= c_i/c \quad (v_i = \pm 1) \end{aligned} \quad (3.28)$$

and shifting to relative distances ($x_{1i} = x_1 - x_i$),

$$\begin{aligned} \widetilde{\Delta f}_n(\tau) &= \widetilde{\Delta f}_n(x_1, x_{12}, \dots, x_{1n}, v_1, \dots, v_n; \tau) \\ &= \Delta f_n(x_1, x_2, \dots, x_n, v_1, \dots, v_n; \tau) \end{aligned} \quad (3.29)$$

[we shall omit the tilde in the equations below; however, it must be clear that the functions $\Delta f_n(\tau)$ refer to the definition (3.29)], we get

$$\begin{aligned} \frac{\partial \Delta f_1(\tau)}{\partial \tau} &= \left(-v_1 \frac{\partial}{\partial x_1} + \bar{C} \right) \Delta f_1(\tau) + \int dx_{12} \sum_{v_2} K_{12} \Delta f_2(\tau) \\ &\vdots \end{aligned} \quad (3.30a)$$

$$\begin{aligned} \frac{\partial \Delta f_n(\tau)}{\partial \tau} &= \left(-v_1 \frac{\partial}{\partial x_1} \cdots - v_{1n} \frac{\partial}{\partial x_{1n}} + \bar{C} \right) \Delta f_n(\tau) \\ &+ \int dx_{1,n+1} \sum_{v_{n+1}} K_{1,n+1} \Delta f_{n+1}(\tau) \end{aligned} \quad (3.30b)$$

where $\bar{C} = (\rho c)^{-1} C$.

3.3. H-Theorem

Because the set of equations (3.30) is linear, it is quite natural to look, as the associated Lyapunov function, for the square of the reduced functions; so let us define

$$H_n(\tau) = \sum_{v_1 \cdots v_n} \int dx_1 dx_{12} \cdots dx_{1n} \Delta f_n^2(\tau) \quad (3.31)$$

where summation and integration are performed over the P_n subspace (i.e., $x_{12} > 0$ for $v_2 = +1$, $x_{12} < 0$ for $v_2 = -1$, and so on). Then the function

$$H(\tau) = \sum_{n=1}^{\infty} H_n(\tau) \quad (3.32)$$

has the property

$$dH(\tau)/d\tau \leq 0 \quad (3.33)$$

The inequality (3.33) reduces to an equality at equilibrium.

We shall prove the inequality (3.33) in the following way: first we suppose that there is no correlation at $t = 0$; then the proof of Eq. (3.33) is trivial and reduces to the Boltzmann case. Then we add pair correlations at $t = 0$ and we prove that the contribution coming from the destruction term for $\Delta f_1(\tau)$ and that of the collision term for $\Delta f_2(\tau)$ compensate, so that the inequality remains valid. One can then add successively higher order initial correlations and continue the argument.

If at $\tau = 0$ all $\Delta f_{n \geq 2}(0) = 0$, then

$$\begin{aligned} \frac{dH(\tau)}{d\tau} &= \frac{dH_1(\tau)}{d\tau} \\ &= 2 \sum_{v_1 = \pm 1} \int_{-\infty}^{+\infty} dx_1 \Delta f_1(\tau) \left(-v_1 \frac{\partial}{\partial x_1} + C \right) \Delta f_1(\tau) \end{aligned} \quad (3.34)$$

$$\begin{aligned} &= -2 \int_{-\infty}^{+\infty} dx_1 \left[\Delta f_1(v_1 = +1, x_1; \tau) \right. \\ &\quad \left. - \Delta f_1(v_1 = -1, x_1; \tau) \right]^2 \leq 0 \end{aligned} \quad (3.35)$$

Suppose now that, at $t = 0$, $\Delta f_2(0) \neq 0$ but $\Delta f_{n \geq 3}(0) = 0$; we have

$$\frac{dH(\tau)}{d\tau} = \frac{dH_1(\tau)}{d\tau} + \frac{dH_2(\tau)}{d\tau} \quad (3.36)$$

where now

$$\begin{aligned} \frac{dH_1(\tau)}{d\tau} &= 2 \sum_{v_1 = \pm 1} \int dx_1 \Delta f_1(\tau) \left(-v_1 \frac{\partial}{\partial x_1} + \bar{C} \right) \Delta f_1(\tau) \\ &\quad + 2 \sum_{v_1, v_2} \int dx_1 dx_{12} \Delta f_1(\tau) K_{12} \Delta f_2(\tau) \end{aligned} \quad (3.37)$$

$$\begin{aligned} &= -2 \int_{-\infty}^{+\infty} dx_1 \left[\Delta f_1(v_1 = +1, x_1; \tau) - \Delta f_1(v_1 = -1, x_1; \tau) \right]^2 \\ &\quad + 2 \int_{-\infty}^{+\infty} dx_1 \left[\Delta f_1(v_1 = +1, x_1; \tau) - \Delta f_1(v_1 = -1, x_1; \tau) \right] \\ &\quad \times \left[\Delta f_2(v_1 = -1, v_2 = +1, x_1, x_{12} = +\eta; \tau) \right. \\ &\quad \left. - \Delta f_2(v_1 = +1, v_2 = -1, x_1, x_{12} = -\eta; \tau) \right] \end{aligned} \quad (3.38)$$

This expression has no definite sign; however, if we combine it with $dH_2(\tau)/d\tau$, which reads

$$\frac{dH_2(\tau)}{d\tau} = 2 \sum_{v_1, v_2} \int dx_1 dx_{12} \Delta f_2(\tau) \times \left(-v_1 \frac{\partial}{\partial x_1} - v_{12} \frac{\partial}{\partial x_{12}} + \bar{C} \right) \Delta f_2(\tau) \quad (3.39)$$

$$\begin{aligned} &= -2 \int dx_1 \left[\Delta f_2^2(v_1 = +1, v_2 = -1, x_1, x_{12} = -\eta; \tau) \right. \\ &\quad \left. + \Delta f_2^2(v_1 = -1, v_2 = +1, x_1, x_{12} = +\eta; \tau) \right] \\ &\quad - 2 \int dx_1 dx_{12} \sum_{v_2} \left[\Delta f_2(v_1 = +1, v_2, x_1, x_{12}; \tau) \right. \\ &\quad \left. - \Delta f_2(v_1 = -1, v_2, x_1, x_{12}; \tau) \right]^2 \end{aligned} \quad (3.40)$$

we obtain

$$\begin{aligned} \frac{dH(\tau)}{d\tau} &= - \int dx_1 \left[\Delta f_1(v_1 = +1, x_1; \tau) - \Delta f_1(v_1 = -1, x_1; \tau) \right]^2 \\ &\quad - \int dx_1 \left[\Delta f_1(v_1 = +1, x_1; \tau) \right. \\ &\quad \left. + \Delta f_2(v_1 = -1, v_2 = +1, x_1, x_{12} = +\eta; \tau) \right. \\ &\quad \left. - \Delta f_1(v_1 = -1, x_1; \tau) - \Delta f_2(v_1 = +1, v_2 = -1, x_1, x_{12} = -\eta; \tau) \right]^2 \\ &\quad - \int dx_1 \left[\Delta f_2(v_1 = -1, v_2 = +1, x_1, x_{12} = +\eta; \tau) \right. \\ &\quad \left. + \Delta f_2(v_1 = +1, v_2 = -1, x_1, x_{12} = -\eta; \tau) \right]^2 \\ &\quad - 2 \int dx_1 \int dx_{12} \sum_{v_2} \left[\Delta f_2(v_1 = +1, v_2, x_1, x_{12}; \tau) \right. \\ &\quad \left. - \Delta f_2(v_1 = -1, v_2, x_1, x_{12}; \tau) \right]^2 \leq 0 \end{aligned} \quad (3.41)$$

If initially $\Delta f_2(0) \neq 0$, $\Delta f_3(0) \neq 0$, but $\Delta f_{n \geq 4}(0) = 0$, then the expression for $dH_2(\tau)/d\tau$, Eq. (3.40), will be modified, because of the influence of $\Delta f_3(0)$, but at the same time its combination with $dH_3(\tau)/d\tau$ will be such that $dH(\tau)/d\tau \leq 0$; and so on. At each step we add the following negative

quantity:

$$\begin{aligned}
 & 2 \sum_{\{v\}} \int_{P_n} dx_1 \cdots dx_{1n} [\Delta f_n(\tau) \bar{C} \Delta f_n(\tau)] \\
 & \quad + \sum_{\{v\}} \int_{P_{n+1}} dx_1 \cdots dx_{1,n+1} \Delta f_n(\tau) K_{1,n+1} \Delta f_{n+1}(\tau) \\
 & \quad + 2 \sum_{\{v\}} \int_{P_{n+1}} dx_1 \cdots dx_{1,n+1} \Delta f_{n+1}(\tau) \left(-v_{1,n+1} \frac{\partial}{\partial x_{1,n+1}} \right) \Delta f_{n+1}(\tau) \\
 & = \sum_{\{v\}} \int_{P_n} dx_1 \cdots dx_{1,n+1} [\Delta f_n(\tau) \bar{C} \Delta f_n(\tau)] \\
 & \quad - \sum_{\{v\}} \int_{P_{n+1}} dx_1 \cdots dx_{1,n+1} [\Delta f_n(v_1 = +1, \dots, \tau) \\
 & \quad + \Delta f_{n+1}(v_1 = -1, \dots, v_{1,n+1} = -1, \dots, x_{1,n+1} = +\eta; \tau) \\
 & \quad - \Delta f_n(v_1 = -1, \dots, \tau) \\
 & \quad - \Delta f_{n+1}(v_1 = +1, \dots, v_{n+1} = +1, \dots, x_{1,n+1} = -\eta; \tau)]^2 \\
 & \quad - \sum_{\{v\}} \int_{P_{n+1}} dx_1 \cdots dx_{1,n+1} \\
 & \quad \times [\Delta f_{n+1}(v_1 = -1, \dots, v_{n+1} = +1, \dots, x_{1,n+1} = +\eta; \tau) \\
 & \quad + \Delta f_{n+1}(v_1 = +1, \dots, v_{n+1} = -1, \dots, x_{1,n+1} = -\eta; \tau)]^2 \quad (3.42)
 \end{aligned}$$

It is also obvious from Eqs. (3.35) and (3.38) that the equilibrium distribution is obtained by requiring $dH(\tau)/d\tau = 0$; it corresponds to

$$\int dx_1 \Delta f_1^{\text{eq}}(v_1, x_1) = \int dx_1 \Delta f_1^{\text{eq}}(-v_1, x_1) \quad (3.43)$$

$$\vdots$$

$$\int dx_1 \Delta f_n^{\text{eq}}(v_1, \dots) = 0 \quad (3.44)$$

One may have a paradoxical situation where the H -function is constant, so that the $\Delta f_n(\tau)$ will have their equilibrium value but some correlations will still exist in the postcollisional subspace, the $\widehat{\Delta f}_n(\tau)$. These correlations do not affect the future values of $\Delta f_n(\tau)$ —which are constant—and will disappear to infinity, simply by free motion and creation of higher order correlations $\Delta f_{m>n}(\tau)$. But consistently they do not produce any entropy in the system.

Because the technical nature of this section may hide the scheme of the proof, we briefly stress some points of the derivation. The set of equations

(3.30) may be written

$$\partial \Delta f / \partial t = \mathbf{M} \cdot \Delta \mathbf{f} \tag{3.45}$$

where the infinite number matrix \mathbf{M} is given by

$$M_{n,n'} = \left[-v_1 \frac{\partial}{\partial x_1} \cdots v_{1,n+1} \frac{\partial}{\partial x_{1,n+1}} + \bar{\mathbf{C}} \right] \delta_{n,n'} + \sum_{v_{n+1}} \int dx_{1,n+1} K_{1,n+1} \delta_{n',n+1} \tag{3.46}$$

contrary to the original hierarchy for $\delta \mathbf{f}$, where another nonvanishing codiagonal $M_{n,n'} \delta_{n',n-1}$ appears. The *H*-function is simply the scalar product $(\Delta f, \Delta f)$ defined by Eqs. (3.31) and (3.32). Because of the infinite sum appearing in Eq. (3.32), we had to prove the inequality (3.33) by a recursive relation [see Eq. (3.42)].

It may appear strange that the free motion operator,

$$-v_{1,n+1} \partial / \partial x_{1,n+1}$$

is essential for the derivation of the *H*-theorem. However, this is related to the decomposition of the phase space and it is not possible to reproduce such a proof for an ideal gas, because of the absence in that case of the dissipative operator $\bar{\mathbf{C}}$.

Let us also mention that we presented an *H*-function which does not depend on the space variable. This is a limitation because we have to suppose, at least at $t = 0$, that the norm is finite. There is, however, no difficulty in defining a local entropy.

4. VELOCITY INVERSION

Let us finally illustrate the results by calculating the *H*-function during a velocity inversion “experiment.” The experiment can be described as follows: we prepare the system at time $-\tau_0$ in a nonequilibrium situation but without any correlation. The system evolves up to time zero, when we invert all particle velocities. Because of the reversibility of laws of motion, the system will evolve backward, recovering its initial state at time $+\tau_0$, except for the inverted velocities. In Ref. 1 we showed that the equation for $\Delta f_1(\tau)$ correctly describes this phenomenon. Also, for a sufficiently short τ_0 , we can limit the study of correlations to binary correlations, that is, $\delta f_2(\tau)$, as there is no time for higher order correlations to be built. Here we shall calculate the *H*-function for a short τ_0 , so that we will be allowed to neglect the $H_{n \geq 3}(\tau)$ in the infinite series for $H(\tau)$.

The initial state is a homogeneous state with no correlations but with a nonequilibrium velocity distribution for the tagged particle. Because the system is homogeneous we shall work with the integral over the x_1 variable

of the reduced distribution function

$$\begin{aligned} \Delta\varphi_n(v_1, \dots, v_n, x_{12}, \dots, x_{1n}; \tau) \\ = \int dx_1 \Delta f_n(v_1, \dots, v_n, x_1, \dots, x_{1n}; \tau) \end{aligned} \quad (4.1)$$

So, at time $-\tau_0$ we have

$$\Delta\varphi_1(v_1 = +1, -\tau_0) - \Delta\varphi_1(v_1 = -1, -\tau_0) = +1 \quad (4.2)$$

$$\Delta\varphi_{n \geq 2}(-\tau_0) = 0 \quad (4.3)$$

(a) Between $\tau = -\tau_0$ and $\tau = 0$. The state of the system is given by the solutions of the kinetic equations [see Eqs. (3.13), (3.21), and (3.23)]:

$$\Delta\varphi_1(v_1, \tau) = \exp[\bar{C}(\tau + \tau_0) \Delta\varphi_1(v_1, -\tau_0)] \quad (4.4)$$

$$\begin{aligned} \widehat{\Delta\varphi}_2(v_1, v_2, x_{12}; \tau) = \int_{-\tau_0}^{\tau} d\tau_1 \exp\left[\left(-v_{12} \frac{\partial}{\partial x_{12}} + \bar{C}\right)(\tau_1)\right] \\ \times K_{12} \Delta\varphi_1(\tau - \tau_1) \end{aligned} \quad (4.5)$$

$$\Delta\varphi_{n \geq 2}(\tau) = 0 \quad (4.6)$$

We have not written down the $\widehat{\Delta\varphi}_{n \geq 3}(\tau)$, which, although they are created by collisions taking place in the system, are negligible because τ_0 has been chosen small.

Using the explicit representation of the propagators in Eqs. (4.4) and (4.5) [see Eq. (3.38) of Ref. 1], we obtain the following expressions for $\Delta\varphi_1(\tau)$ and $\widehat{\Delta\varphi}_2(\tau)$:

$$\Delta\varphi_1(v_1 = +1; \tau) = 1 - \Delta\varphi_1(v_1 = -1; \tau) \quad (4.7)$$

$$= \frac{1}{2}(1 + e^{-2(\tau + \tau_0)}) \quad (4.8)$$

$$\begin{aligned} \widehat{\Delta\varphi}_2(v_1 = v_2 = +1, x_{12}; \tau) \\ = -\widehat{\Delta\varphi}_2(v_1 = v_2 = -1, -x_{12}; \tau) \end{aligned} \quad (4.9)$$

$$\begin{aligned} = e^{-2(\tau + \tau_0)} \int_{-\tau_0}^{\tau} d\tau_1 e^{\tau_1} I_0\left([-x_{12}(2\tau_1 + x_{12})]^{1/2}\right) \\ \times \eta(-x_{12}(2\tau_1 + x_{12})) \end{aligned} \quad (4.10)$$

$$\begin{aligned} \widehat{\Delta\varphi}_2(v_1 = -v_2 = +1, x_{12}; \tau) \\ = -\widehat{\Delta\varphi}_2(v_1 = -v_2 = -1, -x_{12}; \tau) \end{aligned} \quad (4.11)$$

$$\begin{aligned} = e^{-2(\tau + \tau_0)} \left[e^{|x_{12}|/2} + \int_{-\tau_0 + |x_{12}|/2}^{\tau} d\tau_1 e^{\tau_1} \left(\frac{x_{12}}{2\tau_1 - x_{12}} \right)^{1/2} \right. \\ \left. \times I_1\left([x_{12}(2\tau_1 - x_{12})]^{1/2}\right) \eta(x_{12}(2\tau_1 - x_{12})) \right] \end{aligned} \quad (4.12)$$

where $I_n(x)$ are Bessel functions of the first kind⁽¹³⁾ and $\eta(x)$ is the Heaviside function.

(b) At time $\tau = 0$ we invert the velocities of all particles. Let Π be defined by

$$\Pi f(v_1, \dots, v_n) = f(-v_1, \dots, -v_n) \quad (4.13)$$

Then the state after inversion is given by

$$\Delta\varphi_n(\tau = 0^+) = \Pi \widehat{\Delta\varphi}_n(\tau = 0^-) \quad (4.14)$$

$$\widehat{\Delta\varphi}_n(\tau = 0^+) = \Pi \Delta\varphi_n(\tau = 0^-) = 0 \quad (4.15)$$

These last equations show that the inversion of velocities shifts the correlations from the $(1 - P_2)$ subspace to the P_2 subspace; indeed

$$\Pi(1 - P_2) = P_2\Pi \quad (4.16)$$

The system now evolves according to the equations

$$\frac{\delta\Delta\varphi_1}{\delta\tau} = \bar{C}_n \Delta\varphi_1 + \mathfrak{D}_1(\Delta\varphi_n(0t) | \tau) \quad (4.17)$$

$$\frac{\delta\Delta\varphi_2}{\delta\tau} = \left(-v_{12} \frac{\delta}{\delta K_{12}} + \bar{C} \right) \Delta\varphi_2 + \mathfrak{D}_2(\Delta\varphi_n(0t) | \tau) \quad (4.18)$$

In Ref. 1 it was shown that, with the initial condition (4.14), the destruction term $\mathfrak{D}_1(\tau)$ reduces to

$$\mathfrak{D}_1(\tau) = -2\bar{C}\Pi \Delta\varphi_1(-\tau), \quad 0 \leq \tau \leq \tau_0 \quad (4.19)$$

$$= 0 \quad \tau > \tau_0 \quad (4.20)$$

Thus that the solution of Eq. (4.17) is, for $\tau < \tau_0$,

$$\Delta\varphi_1(\tau) = \Pi \Delta\varphi_1(-\tau) \quad (4.21)$$

By the same procedure, it is easy to show that

$$\mathfrak{D}_2(\tau) = -2\bar{C}\Pi \widehat{\Delta\varphi}_2(-\tau), \quad 0 \leq \tau \leq \tau_0 \quad (4.22)$$

$$= 0 \quad \tau > \tau_0 \quad (4.23)$$

and therefore

$$\Delta\varphi_2(\tau) = \Pi \widehat{\Delta\varphi}_2(-\tau) \quad (4.24)$$

At $\tau = \tau_0$ the system has returned to its initial state and starts evolving again according to Eqs. (4.4), (4.5).

(c) The *H*-function, for negative times, is simply the Boltzmann *H*-function, so

$$H(\tau) = H_1(\tau) = \sum_{v_1} \Delta\varphi_1^2(v_1; \tau), \quad -\tau_0 \leq \tau \leq 0 \quad (4.25)$$

$$= \frac{1}{2}(1 + e^{-4(\tau + \tau_0)}) \quad (4.26)$$

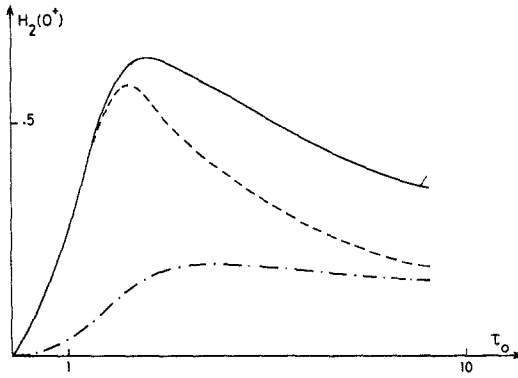


Fig. 2. $H_2(0^+)$ as a function of τ_0 . (- -) Contributions coming from $v_1 = -v_2$. (- · -) Contributions coming from $v_1 = v_2$. (—) Total contribution.

However, for $\tau > 0$, as we have seen, the velocity inversion shifts the correlations to the P_2 subspace, and we have

$$H(\tau) = H_1(\tau) + H_2(\tau) + \dots \tag{4.27}$$

where [see Eq. (4.21)]

$$H_1(\tau) = H_1(-\tau) = \frac{1}{2}(1 + e^{-4(\tau_0 - \tau)}), \quad \tau < \tau_0 \tag{4.28}$$

and [see Eq. (4.24)]

$$H_2(\tau) = \sum_{v_1, v_2} \int dx_{12} \Delta\varphi_2^2(\tau) \tag{4.29}$$

$$= \sum_{v_1, v_2} \int dx_{12} \widehat{\Delta\varphi}_2^2(-\tau) \tag{4.30}$$

whereas $H_3(\tau)$ is negligible as long as we maintain τ_0 small [this can be checked by a short-time expansion of $\Delta\varphi_3(\tau)$].

In Fig. 2 we show the jump of the H -function at $\tau = 0$ as a function of

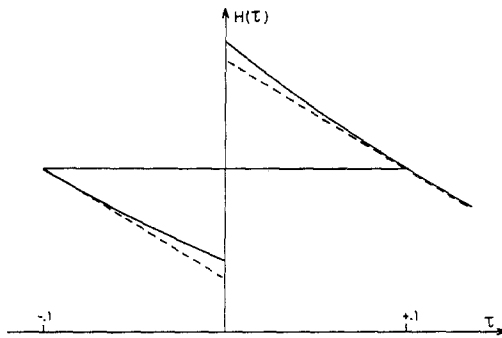


Fig. 3. The H -function expanded in powers of τ ($\tau_0 = 0.1$). (- -) Order τ ; (—) order τ^2 .

τ_0 ; this figure clearly shows that this jump is important for short τ_0 . For long τ_0 one needs to look for higher order correlations to get the jump for the *H*-function. The distinction we make between contributions to $H_2(\tau = 0^+)$ coming from configurations with opposite and those with equal velocities shows that the short-time behavior is dominated by free motion, whereas the long-time behavior is a diffusive process, so that the two contributions have equal importance.

Figure 3 shows a short-time expansion of $H(\tau)$ during the all velocity inversion experiment, neglecting terms of the order τ^3 and putting $\tau_0 = 0.1$.

5. CONCLUDING REMARKS

The main result of this paper is a definition of an *H*-function (or an entropy) which depends on nonequilibrium correlations. It is based on a peculiarity of this one-dimensional model, namely the existence of projections of the reduced distribution functions which obey a closed system of kinetic equations. This decoupling depends on the correlations initially present. The time evolution of these correlations is dissipative and the system goes to equilibrium. The construction proposed for the *H*-function depends on this property and is in no way general. However, it shows how a dynamical system may, in the thermodynamic limit, behave dissipatively.

Another point of interest is that one has to go to a reduced description before defining the *H*-function. This reduction seems to be necessary in order to distinguish between a simple "phase mixing" evolution, as happens in an infinite ideal gas, and an approach to equilibrium with a well-defined transport coefficient, as appears in the model studied here—up to now, the reduction seems to be an inescapable restriction.

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