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H Theorem for the (Modified) Nonlinear Enskog Equation

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I construct an entropy function $S(t)$ suitable for a system of hard spheres satisfying the (modified) nonlinear Enskog equation, and show that $\partial_t S(t) \geq 0$. The equality sign holds only when the system has reached absolute equilibrium, in which case S becomes the exact equilibrium entropy of the hard-sphere fluid.

Despite its phenomenological character, the Enskog equation[1-3] is quite successful in describing transport phenomena in dense fluids.[4] This equation, governing the time evolution of the one-particle distribution function (d.f.) $f_1(\vec{r}_1, \vec{v}_1; t)$, is written

$$\partial_t f_1 + \vec{v}_1 \cdot \frac{\partial}{\partial \vec{r}_1} f_1 = J^E(f_1, f_1), \tag{1}$$

where the collision operator J^E is defined by

$$J^E(f_1,f_1) = a^2 \int d^3v_2 \int d^2\epsilon\, \vec{\epsilon}\cdot\vec{v}_{12}\, \theta(\vec{\epsilon}\cdot\vec{v}_{12})\, [g_2(\vec{r}_1, \vec{r}_1 - a\vec{\epsilon}\,|n) f_1(\vec{r}_1, \vec{v}_1'; t) f_1(\vec{r}_1 - a\vec{\epsilon}, \vec{v}_2'; t) - g_2(\vec{r}_1, \vec{r}_1 + a\vec{\epsilon}\,|n) f_1(\vec{r}_1, \vec{v}_1; t) f_1(\vec{r}_1 + a\vec{\epsilon}, \vec{v}_2; t)]. \tag{2}$$

Here, a denotes the hard-sphere diameter, $\vec{\epsilon}$ is a unit vector, and $\theta(x)$ is the Heaviside function; moreover, $\vec{v}_1'$ and $\vec{v}_2'$ are the velocities after the collision and g_2, a functional of the density $n(\vec{r}; t)$, is defined presently.

In his original intuitive argument, Enskog took for g_2 the equilibrium pair correlation at contact, calculated for the local density at point $\frac{1}{2}(\vec{r}_1 + \vec{r}_2)$. Yet, more recent investigations[5,6] indicate that this proposal has to be slightly modified in order to lead to a consistent theory (which, in particular, should be compatible with Onsager relations). These works lead to a systematic derivation of this (modified) Enskog theory from the *single assumption* that, for all times, the N-particle distribution function of the system takes the form

$$\rho_N(\vec{r}_1, \ldots, \vec{r}_N, \vec{v}_1, \ldots, \vec{v}_N; t) = \prod_{i>j=1}^{N} \theta_{ij} \prod_{i=2}^{N} W_1(\vec{r}_i, \vec{v}_i; t)/\Phi_0(t) \tag{3}$$

when N (and the volume of the system Ω) becomes large. Here $\theta_{ij} \equiv \theta(r_{ij} - a)$ takes into account the excluded volume between the pair of spheres i, j and $\Phi_0(t)$ is the factor normalizing ρ_N. Obviously, the crucial assumption in (3) is that the velocity dependence of ρ_N enters only through the one-body function W_1. This latter quantity is *defined* in such a way that f_1, as calculated from (3), is that realized by the dynamical equation (1). Albeit exact at equilibrium (where W_1 becomes the Maxwellian), (3) can only be approximately true for all times.

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From the *Ansatz* (3), the reduced d.f. f_2, g_2, etc., can be computed in the usual way[3]; in particular, one obtains a well-defined expression for the pair correlation g_2, which depends on time through the density $n(\vec{r};t)$ only, and one also proves that g_2 satisfies the relation

$$f_2(\vec{r}_1,\vec{v}_1,\vec{r}_2,\vec{v}_2;t) = g_2(\vec{r}_1,\vec{r}_2|n)f_1(\vec{r}_1,\vec{v}_1;t)f_1(\vec{r}_2,\vec{v}_2;t) \tag{4}$$

which, when inserted into the first Bogoliubov-Born-Green-Kirkwood-Yvon equation, precisely leads to the Enskog equation [(1) and (2)], now called "modified" because of the new definition of g_2.[7]

The aim of the present Letter is to point out that an H theorem, very similar to Boltzmann's result for dilute gases, is valid for this modified Enskog equation. This result furnishes the first example of an explicit proof of the approach to equilibrium of a strongly interacting system.[8]

I start by *defining* the nonequilibrium entropy by $S(t) = -k_B\int d^3r_1\cdots d^3r_N d^3v_1\cdots d^3v_N\, \rho_N(t)\ln\rho_N(t)$, where ρ_N is *given* by Eq. (3).[9] This entropy is a functional of f_1 only; indeed, it can be decomposed ($S = S' + S''$) into a "kinetic" part

$$S' = -k_B\int d^3r_1 d^3v_1\, f_1(\vec{r}_1,\vec{v}_1;t)\ln f_1(\vec{r}_1,\vec{v}_1;t) \tag{5}$$

and a "potential" part

$$S'' = -k_B[\ln\Phi_0(n) + \int d^3r_1\, n(\vec{r}_1;t)\ln a_1(\vec{r}_1;t)], \tag{6}$$

where the normalizing factor Φ_0 [see (3)] and the function a_1 defined by

$$a_1(\vec{r}_1|n) \equiv f_1(\vec{r}_1,\vec{v}_1;t)/W_1(\vec{r}_1,\vec{v}_1;t) \tag{7}$$

[a_1 is independent of $\vec{v}_1$; see (3)] depend on time through $n(\vec{r};t)$ only.

Using a series of manipulations usual in hard-sphere dynamics,[2,3] one shows that

$$\partial_t S' = -\tfrac{1}{2}k_B a^2\int d^3r_1\, d^3r_2\, d^3v_1\, d^3v_2\int d^2\epsilon\,(\vec{\epsilon}\cdot\vec{v}_{12})\theta(\vec{\epsilon}\cdot\vec{v}_{12})g_2(\vec{r}_1,\vec{r}_2|n(t))\delta(\vec{r}_{12}+a\vec{\epsilon})f_{1,1}f_{1,2}\ln\left(\frac{f_{1,1}f_{1,2}}{f_{1,1'}f_{1,2'}}\right) \tag{8}$$

with, for example, the abreviation $f_{1,2'} \equiv f_1(\vec{r}_2,\vec{v}_2';t)$, etc.

With the inequality $x\ln(x/y) \geq x - y$ (where $x = f_{1,1}f_{1,2} > 0$ and $y = f_{1,1'}f_{1,2'} > 0$), I obtained from (8) the inequality $\partial_t S' \geq I$, with (to simplify I have used periodic conditions at the boundaries)

$$I = -k_B\int d^3r_1\, d^3r_2(\vec{r}_{12}/a)\delta(r_{12}-a)g_2(\vec{r}_1,\vec{r}_2|n)\cdot[\int d^3v_1\,\vec{v}_1 f_1(\vec{r},\vec{v}_1;t)]n(\vec{r}_2;t). \tag{9}$$

Notice that the equality only holds if

$$f_1(\vec{r}_1,\vec{v}_1;t)f_1(\vec{r}_1+a\vec{\epsilon},\vec{v}_2;t) = f_1(\vec{r}_1,\vec{v}_1';t)f_1(\vec{r}_1+a\vec{\epsilon},\vec{v}_2';t) \tag{10}$$

for all $\vec{r}_1,\vec{v}_1,\vec{v}_2,\vec{\epsilon}$ such that $\vec{\epsilon}\cdot\vec{v}_{12} > 0$.

The potential entropy S'', functionally depending on the density, has its time behavior governed by the continuity equation. Using the definition of Φ_0 and a_1, one finds precisely $\partial_t S'' = -I$. Therefore,

$$\partial_t S \geq 0. \tag{11}$$

Finiteness of particle density and of kinetic energy density[6] suffices to show that asymptotically $\partial_t S = 0$ ($t\to\infty$) and one proves from (10) that f_1 then reaches absolute equilibrium.

Despite the approximate nature of the modified Enskog equation (in particular, its Markovian character), my result indicates that the original Boltzmann ideas still remain valuable in describing the approach to equilibrium of f_1 in strongly interacting systems: My definition of entropy is the simplest generalization of the dilute-gas expression (formally obtained by setting $\theta_{ij} = 1$, and thus $S'' = \text{const}$) which leads to the exact equilibrium entropy; yet, it obeys an H theorem.

[1]D. Enskog, K. Sven. Vetenskapakad. Handl. 4, 63 (1922).

[2]S. Chapman and T. Cowling: *The Mathematical Theory of Non-Uniform Gases* (Cambridge Univ. Press, Cambridge, 1935).

[3]For more recent presentations, see P. Résibois and M. De Leener, *Classical Kinetic Theory of Fluids* (Wiley,

New York, 1977); J. Dorfman and H. van Beijeren, in *Statistical Mechanics*, edited by B. Berne (Plenum, New York, 1977), Part B.

[4]For review see H. Hanley, R. MacCarthy, and E. Cohen, Physica (Utrecht) 60, 322 (1972); J. Piasecki in "Fundamental Problems in Statistical Mechanics," edited by E. Cohen (to be published); P. Résibois, *ibid.*

[5]J. Lebowitz, J. Percus, and J. Sykes. Phys. Rev. 188, 487 (1967); J. Sykes: J. Stat. Phys. 8, 279 (1973).

[6]H. van Beijeren and M. Ernst, Physica (Utrecht) 68, 437 (1973), and 70, 225 (1973).

[7]As shown in Refs. 5 and 6, this modification is of second order in the gradients $[\propto(\partial/\partial\vec{r}_1)^2]$ for a simple gas; therefore, it does not affect the transport coefficients. Yet, for *arbitrary* f_1, the following is not applicable to the original Enskog equation.

[8]For an interesting approach at the level of N-body master equations, see I. Prigogine, C. George, F. Henin, and L. Rosenfeld, Chem. Scr. 4, 5 (1973).

[9]Of course, exactly as in the dilute-gas limit, if ρ_N was the exact d.f., $S(t)$ would remain constant [see, for example, S. Rice and P. Gray, *The Statistical Mechanics of Simple Liquids* (Interscience, New York, 1965)]; the use of the approximate ρ_N, Eq. (3), is just a trick to *define* $S(t)$ in terms of f_1 (or W_1); since this latter function (and not for the exact ρ_N) is an irreversible behavior *a priori* expected.

Screening Solutions to Classical Yang-Mills Theory

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We present two new solutions to the classical Yang-Mills field equations in the presence of a localized external source. These solutions totally screen the charge of the source. They have lower energy than the corresponding Coulomb solution.

Non-Abelian gauge theories offer the greatest promise to describe the elementary forces in nature. We here investigate the solutions to the classical Yang-Mills equations in the presence of a static external source in Minkowski space:

$$(D_\mu F^{\mu\nu})^a = j^{a\nu}(x) = \delta^{\nu 0} q^a(x), \tag{1a}$$

$$F_{\mu\nu}{}^a = \partial_\mu A_\nu{}^a - \partial_\nu A_\mu{}^a + g c^{abc} A_\mu{}^b A_\nu{}^c, \tag{1b}$$

where $q^a(x)q^a(x)$ is time independent. By a local gauge transformation, one can always line up the source into commuting directions of color space, e.g., $q^a(x) \to \delta^{a3}[q^b(x)q^b(x)]^{1/2} = \delta^{a3}q(\vec{x})$ for SU(2) which for simplicity we will study first. The *Ansatz*[1] $A_\mu{}^a = \delta^{a3}A_\mu$ then reduces Eqs. (1) to the Maxwell equations of electrodynamics. We call the corresponding solution the Coulomb solution for the source $q^a(x)$.

However, various results in the literature have already shown that classical unbroken Yang-Mills theories in Minkowski space are qualitatively different from electrodynamics, e.g., the Wu-Yang monopole[2] and Coleman's non-Abelian plane wave[3] which are both nontrivial solutions to Eqs. (1) with $q^a(x) = 0$. Moreover, Mandula[4] has shown that the Coulomb solution corresponding to a static source distributed over a thin spherical shell is unstable if $gQ > \frac{3}{2}$, where $Q = \int d^3x[q^a(x)q^a(x)]^{1/2}$. Mandula also showed that the instability modes produce an inward flow of charge that tends to screen the external source. Since the energy is positive definite, Eqs. (1) must admit static solutions of lower energy than the Coulomb one. Below we exhibit two new types of solutions to Eqs. (1) with localized and integrable static sources. The first type has the long-range behavior of a magnetic dipole field, and has lower energy than the Coulomb solution once gQ is large enough. The second type has no long-range field strengths at all, and its energy can be made arbitrarily small.

The magnetic dipole solution.—The *Ansatz*

$$\begin{aligned} &A_0{}^1 = A_0{}^2 = A_i{}^2 = A_i{}^3 = 0, \\ &A_0{}^3 = \varphi(\rho, x_3), \quad A_i{}^1 = \epsilon_{i3j}(x_j/\rho)A(\rho, x_3), \end{aligned} \tag{2}$$

where $\rho = [x_1{}^2 + x_2{}^2]^{1/2}$, assures that all the Eqs. (1) are automatically satisfied provided

$$-\nabla^2\varphi + g^2A^2\varphi = q, \tag{3a}$$

$$+\nabla^2 A - \rho^{-2}A + g^2\varphi^2 A = 0. \tag{3b}$$

The Coulomb solution corresponds to setting $A = 0$. Outside of this *Ansatz*, the full nonlinearity of the equations comes into play and there are no analytical methods available. It is nevertheless

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