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ON A DERIVATION OF THE BOLTZMANN EQUATION

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My objective in this exposition is to motivate, state, and explain a theorem which says that the Boltzmann equation gives an approximate discription of the behavior a system of classical particles interacting by short range forces, which description becomes exact in the limit as the number of particles becomes infinite and the range of the interparticle forces goes to zero. I will not discuss the proof of the theorem; it is outlined in [1]. I have tried to make my explanations as detailed and elementary as possible, and I apologize to the reader who finds them too detailed. I apologize also for the lack of an adequate bibliography; failure to cite other work in this field is not to be interpreted as meaning that I find it irrelevant or unimportant. (The volume containing [3] is a good place to look for a comprehensive survey of work related to the Boltzmann equation.) Finally, I should warn the practical-minded reader at the outset that the theorem to be stated says only that the Boltzmann equation holds for times no larger than one-fifth of a mean free time and hence does not suffice to justify its physically interesting applications.

The conceptual foundations of the Boltzmann equation seem to me to merit careful study not so much for their own sake as because the Boltzmann equation is a prototype of a mathematical construct central to the theory of time-dependent phenomena in large systems - a reduced or "macroscopic" description taking into account only partial

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information about the underlying microscopic state but nevertheless undergoing an autonomous time development. Very schematically, the idea is to isolate some of the co-ordinates of the manifold of all microscopic states which are, at least in an idealized sense, accessible to macroscopic measurement. These co-ordinates are coupled, in the exact equations of motion, to the other less accessible co-ordinates. Thus, the values of the macroscopic co-ordinates at one time do not determine their values at later times, i.e., the macroscopic co-ordinates do not undergo an autonomous time evolution. Nevertheless, as the number of particles increases to infinity, so the microscopic description becomes more and more intricate, one can hope that the effect of the non-macroscopic co-ordinates on the macroscopic ones becomes, statistically, a function of the macroscopic co-ordinates themselves so that in the limit the macroscopic co-ordinates determine their own time evolution. The theorem we are going to formulate will say that something like this does indeed happen, but it applies only to a particular limiting situation representing an infinitely dilute gas. It is the fact that the density is vanishingly small which makes the analysis feasible; obtaining generalizations which apply to matter at non-zero density is perhaps the central problem of non-equilibrium statistical mechanics.

The above paragraph hints that there is some element of probabilistic reasoning involved in the passage from the microscopic to the macroscopic description. This is in fact the case, but the use made of probabilistic ideas is more subtle than might be expected In particular the point of view to be developed is not that the Boltzmann equation holds "on the average" but rather that it gives an accurate description of the time development of "almost all" initial

points. The selection of a minimal set of probabilistic assumptions permitting the above statement to be made precise remains one of the least satisfactory aspects of the theory.

With these remarks by way of introduction, I want next to give a brief account of the heuristic reasoning leading to the Boltzmann equation, following reasonably closely Boltzmann's original argument. One starts from the following picture of what is happening at the molecular level: The piece of matter under investigation is made up of a large number of particles (molecules) moving according to the laws of classical mechanics and interacting with each other by a short range two-body potential. (The results to be described here were originally proved for a system of hard spheres interacting only by elastic collision [1], but most of them have now been extended to general finite range non-negative potentials [2].) We assume the density to be low so that each particle moves freely most of the time but occasionally undergoes a collision with another particle in which its velocity changes very quickly. The state of the system is specified at any time by giving the positions and velocities of all the particles:

$$(\vec{q}_1, \vec{v}_1; \ldots; \vec{q}_n, \vec{v}_n) \ ;$$

the state at any other time is determined "simply by solving the equations of motion". Of course, for n of the order of 10^{23} this is hard to do.

Boltzmann therefore approached the time-evolution problem from a different direction. Instead of specifying the initial state by giving the positions and velocities of all the particles, one can instead specify a discrete mass distribution on the one-particle phase space $\Lambda \times R^3$ (where $\Lambda \subset R^3$ is the region in which the

material is localized); this mass distribution can even be assumed normalized. (More explicitly, we may represent $(\vec{q}_1,\vec{v}_1;\ldots;\vec{q}_n,\vec{v}_n)$ by $\frac{1}{n}\sum_{i=1}^{n}\delta_{\vec{q}_i,\vec{v}_i}$.) It is reasonable to expect, given the large value of n, that this mass distribution will be well approximated by a "continuous" mass distribution

$$f(\vec{q},\vec{v})d\vec{q}\,d\vec{v}$$

Boltzmann proposed to write down the equation of motion directly in terms of the function f.

The idea of describing an n-particle phase point by a continuous mass distribution has a somewhat paradoxical character. On the one hand, it is intuitively a very sensible thing to do, given the large value of n. On the other hand, it is qualitatively completely incorrect if looked at closely, since the true mass distribution is after all discrete for any finite n. Therefore, if one wants to use this description to make exact statements, one is forced to pass to the limit $n \to \infty$. At this point, a natural kind of macroscopic description arises. Physically, what is intended is something like this: One cuts up the one-particle phase space into a large number of small but finite cells, and instead of specifying the exact position and velocity of each particle, one specifies the state of the system approximately by giving the number of particles in each cell. If the cells are small enough (e.g., comparable in size to the molecules themselves), then the approximate description contains almost as much information as the exact description. We want to look instead at the opposite limiting situation where the number of particles is much larger than the number of cells, so that the occupation numbers give a description which is far from complete. One could now make a precise, if excessively special, definition of

"macroscopic description" by choosing at the outset a partition of the one particle phase space into a finite number of cells, declaring the occupation numbers of those cells to be the macroscopic observables and asking what can be said about the time development of this macroscopic description in the limit $n \to \infty$. This program can be carried out, using the general theorem to be formulated here, but it has at least two drawbacks:

a. It seems excessively restrictive to make the theory depend on a particular choice of the decomposition of the one-particle phase space into cells.

b. The evolution equations for a finite number of occupation numbers have technically unpleasant features (specifically are non-Markovian) which disappear if the cells are allowed to become "infinitesimal".

Thus, superimposed on the fundamental limit $n \to \infty$, there is a secondary limit in which the size of the cells goes to zero. This second limit must, however, be taken after, or more slowly than, the limit $n \to \infty$. Intuitively, the cells are to be taken small enough to be treated as infinitesimal from the macroscopic point of view but big enough so that each of them contains a large number of particles.

Let us now forget temporarily the logical subtleties involved in describing microscopic states by continuous distributions $f(\vec{q},\vec{v})$ and continue with the heuristic derivation of the equation of motion for f. Since $nf(\vec{q},\vec{v})d\vec{q}\ d\vec{v}$ is the number of particles in a given infinitesimal cell in the one-particle phase space, the change of f with time may be deduced from knowing how the positions and velocities of the particles change. We have already said that we are considering a low-density regime in which particles mostly move

in straight lines with uniform velocities but occasionally undergo collisions in which their velocities change (almost) discontinuously. The contribution of the uniform rectilinear motion to the change in f with time is simple to write down, but the collision contribution requires more ingenuity. Basically what one needs to know is the fraction of particles with approximate position $\vec{q}_0$ and approximate velocity $\vec{v}_0$ which, in time dt, undergo collision with another particle with approximate velocity $\vec{v}_1$ giving collision products velocities $\vec{v}_0', \vec{v}_1'$. It is not apparent that this fraction is actually a function of the occupation numbers alone. Nevertheless, Boltzmann proposed the following prescription: Consider the one-particle probability distribution $f(\vec{q}_1,\vec{v}_1)d\vec{q}_1 d\vec{v}_1$. Compute the probability with respect to this distribution that a test particle at $(\vec{q}_0,\vec{v}_0)$ undergoes a collision of the indicated kind. Multiply this probability by the total number n of particles present to get the desired fraction. Using this prescription, together with some straightforward manipulations, he wrote down his equation for the time development of f. (This is actually not quite correct; the above derivation leads to a slightly more complicated equation, called the Enskog equation. To get the Boltzmann equation, it is necessary to make the further approximation of neglecting changes in f when $\vec{q}$ changes by an amount of the order of the range of the intermolecular force.)

The outcome of this calculation, for a system of n spheres of diameter d, is

$$\frac{d}{dt}f_t(\vec{q},\vec{v}) =$$

$$\vec{v}\cdot\frac{\partial}{\partial\vec{q}}f_t(\vec{q},\vec{v}) + nd^2\int_{R^3} d\vec{v}_1 \int d\hat{\omega}\ \hat{\omega}\cdot(\vec{v}-\vec{v}_1)\{f_t(\vec{q},\vec{v}_1')f_t(\vec{q},\vec{v}') - f_t(\vec{q},\vec{v}_1)f_t(\vec{q},\vec{v})\}$$

where the $\hat{\omega}$ integral denotes the surface integral over the hemisphere

$\{\hat{\omega}: |\hat{\omega}| = 1, \hat{\omega}.(\vec{v}-\vec{v}_1) \geq 0\}$ and where

$$\vec{v}_1' = \vec{v}_1 + \hat{\omega}.[\hat{\omega}.(\vec{v}-\vec{v}_1)]$$

$$\vec{v}' = \vec{v} - \hat{\omega}.[\hat{\omega}.(\vec{v}-\vec{v}_1)]$$

are the outgoing momenta after a collision with incoming momenta $\vec{v}_1, \vec{v}$ and momentum transfer in the direction $\hat{\omega}$.

For the heuristic reasoning leading to the Boltzmann equation to have any chance of being accurate, the system must satisfy a number of conditions. It is necessary first of all that each infinitesimal cell contain a large number of particles; hence that the number n of particles be large and the diameter d of each particle be small. It is also necessary that the effects of collisions be neither too large nor too small, i.e., that the probability of a typical particle's undergoing a collision in unit time be neither zero nor one. This means that the mean free path should be of order one. To estimate the mean free path λ we argue that the volume of a circular cylinder with height λ and base of radius d should on the average contain one particle:

$$\pi d^2 \lambda \simeq \frac{v(\Lambda)}{n} \; ; \quad \lambda = \frac{v(\Lambda)}{\pi n d^2}$$

so we want to keep nd^2 of order one as we pass to the limit $n \to \infty$, $d \to 0$. We will refer to the limit $n \to \infty$, $d \to 0$, nd^2 approaching a finite non-zero limit, as the Boltzmann-Grad limit. Note that this limit implies $nd^3 \to 0$, which means that the total volume actually occupied by the particles goes to zero and thus that the density should be regarded as approaching zero in spite of the fact that the number of particles in a fixed volume Λ goes to infinity. Note also that n and d appear in the Boltzmann equation only in the combination nd^2, so the equation does make sense in the Boltzmann-Grad limit.

The Boltzmann equation has had a remarkable history of successes in theoretical physics. Boltzmann originally introduced it as the essential element in a proof that an arbitrary velocity distribution for a dilute gas converges as $t \to \infty$ to the Maxwell-Boltzmann distribution. Hilbert, Chapman and Enskog showed that the equations of hydrodynamics can be derived from it. On a more mundane level, it is one of the most important tools in practical gas-dynamics calculations. Despite these successes, it is beset by a number of problems. Its mathematical properties remain obscure and in particular no satisfactory global existence theorem has been proved. Moreover, even from the point of view of theoretical physics, it has the paradoxical feature of being irreversible although it should in principle be derived from the reversible equations of microscopic dynamics. Concretely, this means the following: If $(\vec{q}_1(t),\vec{v}_1(t);\ldots;\vec{q}_n(t),\vec{v}_n(t))$ is a solution of the microscopic equations of motion, then so is $(\vec{q}_1(-t),-\vec{v}_1(-t);\ldots;\vec{q}_n(-t),-\vec{v}_n(-t))$. Intuitively, if all velocities are reversed at some instant of time and the system is then allowed to run normally, it will retrace its previous trajectory backwards. One is thus led to expect that if $f_t(\vec{q},\vec{v})$ is a solution of the Boltzmann equation then so is $f_{-t}(\vec{q},-\vec{v})$. This, however, is definitely false except in trivial cases. We will return later to the question of how our theorem avoids this apparent paradox.

As a first step in formulating a theorem asserting the validity of the Boltzmann equation, we need to make precise the notion that a phase point

$$\underline{x} = (\vec{q}_1,\vec{v}_1;\ldots;\vec{q}_n,\vec{v}_n)$$

is well approximated by a continuous distribution $f(\vec{q},\vec{v})$. A good way to do this is to represent all phase points $\underline{x}$ for all n, as well as continuous distributions like f, as points of a single

space equipped with an appropriate topology. For our purposes, a convenient space is the set of all probability measures υ on $\Lambda \times \mathbb{R}^3$ such that

$$\int \vec{v}^2 \upsilon(d\vec{q}\, d\vec{v}) < \infty .$$

A phase point $\underline{x}$ is represented by

$$\upsilon_{\underline{x}} = \frac{1}{n} \sum_i \delta_{\vec{q}_i, \vec{v}_i}$$

and a density f by the measure $f(\vec{q},\vec{v})d\vec{q}\, d\vec{v}$. The topology we use is the weak*-topology for measures strengthened by requiring that the mapping

$$\upsilon \to \int \vec{v}^2 d\upsilon$$

be continuous. This topology may be described in more intuitive terms as follows: Let n_j be a sequence of integers approaching infinity, and for each j let $\underline{x}_j$ be an n_j-particle phase point. Then $\upsilon_{\underline{x}_j}$ converges to f if and only if:

1. The kinetic energy of $\underline{x}_j$ divided by n_j approaches $\frac{m}{2} \int \vec{v}^2 d\upsilon$
2. For each 6-dimensional rectangle Δ in $\Lambda \times \mathbb{R}^3$, the fraction of particles of $\underline{x}_j$ which are in Δ converges to $\int_\Delta f(\vec{q},\vec{v})d\vec{q}\, d\vec{v}$.

as $j \to \infty$. We will, when convenient, fail to distinguish between $\underline{x}$ and $\upsilon_{\underline{x}}$; thus, we will say $\underline{x}$ is near to f (rather than that $\upsilon_{\underline{x}}$ is near f).

With this terminology, we can formulate a first, overly optimistic, guess about what the connection between the Boltzmann equation and microscopic dynamics might be:

Preliminary Conjecture: If $t > 0$ and if $\underline{x}$ is near f then $T^t\underline{x}$ is near f_t , the solution of the Boltzmann equation with initial value f .

(Here $T^t\underline{x}$ denotes the solution of the exact microscopic equations

of motion with initial condition $\underline{x}$. In formulating the conjecture we have not needed to require explicitly that the number of particles be large; this is implied by the condition that $\underline{x}$ is near f.)

This conjecture is definitely false. This may be seen either by constructing explicit counterexamples (which is not difficult to do) or by observing that it is inconsistent with the fact that the microscopic equations of motion are reversible while the Boltzmann equation is not. It is, however, reasonably close to the truth which is that if $\underline{x}$ is near to f then $T^t\underline{x}$ is very likely to be near f_t, at least for small positive t.

The question is: What is meant by "very likely"? To give this phrase a meaning in a straightforward way, we should start with some probability measure μ on the microscopic state space $(\Lambda \times \mathbb{R}^3)^n$ which is concentrated on (i.e., assigns probability nearly one to) the set of $\underline{x}$'s near f and proceed to show that μ assigns probability very near to one to the set of $\underline{x}$'s such that $T^t\underline{x}$ is near f_t. What μ (or class of μ's) should we start with? One reasonable procedure would be to imitate the microcanonical prescription in equilibrium statistical mechanics, i.e., to construct μ by giving equal weight with respect to ordinary $6n$ dimensional volume to all $\underline{x}$'s which approximate f within a given tolerance and assigning measure zero to the set of all $\underline{x}$'s which do not so approximate f. One is thus led to formulate the following:

Pre-Theorem: Let $t \to f_t$ be a solution of the Boltzmann equation (with a given value of nd^2). For sufficiently small positive t and any neighbourhood V of f_t there is a neighbourhood W of f such that, as $n \to \infty$ with nd^2 fixed,

$$\{\underline{x} \in W \cap (\Lambda \times \mathbb{R}^3)^n : T^t\underline{x} \in V\}$$

forms a fraction arbitrarily close to one of the volume of $W \cap (\Lambda \times \mathbb{R}^3)^n$.

In less precise language, among these $\underline{x}$'s which are close to f, the overwhelming majority with respect to $6n$ dimensional volume have $T^t\underline{x}$ close to f_t;

I have labelled this statement as a pre-theorem rather than a theorem because a number of technical restrictions (notably, some assumptions on the decrease of f at infinity) are necessary to make it correct.

While statements like the above, based on a sort of microcanonical prescription, have the adventage of simplicity, they leave open the fundamental question of justifying the microcanonical prescription. This question is part of the general problem; which may be called the problem of a priori microscopic probabilities, of deciding which probability measure on the microscopic phase space to use to describe a given macroscopic situation. This problem arises already in equilibrium statistical mechanics; even in that simpler situation it is in my opinion far from being resolved. The best one is able to do there is to show that in the limit as the number of particles becomes infinitely large the results obtained depend relatively little on the details of the choice of microscopic probabilities. For example, an important element in the foundations of equilibrium statistical mechanics is the fact that, provided one is careful about what happens at phase-transition points, one obtains the same results by calculating with the canonical or grand canonical ensemble as with the microcanonical ensemble. We will proceed in a similar fashion. Rather than restricting our attention to the microcanonical μ, we will instead formulate a general result giving sufficient conditions under which an initial μ assigns high probability to $\underline{x}$ for which $T^t\underline{x}$ is near f_t; it will then be necessary to come back at the end and verify that an approximate microcanonical prescription gives initial

μ's which do satisfy the hypotheses of the general theorem.

We want, therefore, to formulate a result of the following sort: Given an initial one-particle distribution f and a solution f_t of the Boltzmann equation with initial condition f and a given value of nd^2, if μ is a probability measure on the microscopic phase space for n elastic spheres of diameter d, where n is large, d small, and nd^2 equal to the value appearing in the Boltzmann equation, and if

a) μ assigns high probability to the set of $\underline{x}$'s near f.

b) μ satisfies some further conditions to be formulated shortly

then μ assigns high probability to the set of $\underline{x}$'s such that $T^t\underline{x}$ is near f_t. Even this informal statement is uncomfortably complicated; the statement of a precise theorem along these lines would be almost totally impenetrable. It is therefore convenient to talk in terms of sequences rather than neighbourhoods; this leads to more transparant statements which can, if desired, be translated back in the standard elementary way into the above language. We will accordingly consider as fixed for the next few paragraphs:

a. a sequence of d's (positive real numbers) approaching zero

b. a sequence of n's (positive integers) approaching infinity, such that nd^2 approaches a finite non-zero limit

c. a solution $t \to f_t$ of the Boltzmann equation with the limiting value of nd^2, this solution being assumed to be defined on an interval $[0,\tau]$ of positive times.

d. a sequence of probability measures μ on $(\Lambda \times \mathbb{R}^3)^n$

In principle we should use an index to label these sequences, i.e., we should write d_k, n_k, μ_k, etc. To avoid being overwhelmed by subscripts, however, we will suppress these indices. Whenever d and n appear in the same expression, it is to be understood that

they refer to the same term in the sequence, e.g. nd^2 should be read as $n_k d_k^2$. Similarly, instead of labelling the measures μ with subscripts, we will label them with the corresponding value of d , i.e., we write $\mu^{(d)}$ instead of μ_k .

We must next define what we mean by the statement that a sequence of such probability measures $\mu^{(d)}$ becomes concentrated (as d approaches zero) on the set of microscopic phase points arbitrarily near a given continuous distribution f . If Δ is any subset of the one-particle phase space $\Lambda \times \mathbb{R}^3$, we let F_Δ denote the function on the n-particle phase space $(\Lambda \times \mathbb{R}^3)^n$ which gives the fraction of particles which lie in Δ , viz., for $\underline{x} = (q_1,v_1;\ldots;\vec{q}_n,\vec{v}_n)$,

$$F_\Delta(x) = \frac{1}{n} \sum_{i=1}^{n} \chi_\Delta(\vec{q}_i,\vec{v}_i) \ ,$$

where χ_Δ is the characteristic function of Δ . Although F_Δ actually stands for a sequence of functions (one for each n), we have suppressed the n dependence from the notation as we want to think of F_Δ's with different values of n as representing "the same" measurement made on different systems. We will say that a sequence $\mu^{(d)}$ of probability measures on $(\Lambda \times \mathbb{R}^3)^n$ is an <u>approximating sequence</u> for f if, for each rectangular parallelipiped Δ in $\Lambda \times \mathbb{R}^3$, the random variable F_Δ on the probability space $((\Lambda \times \mathbb{R}^3)^n,\mu^{(d)})$ converges in distribution as $d \to 0$ to the constant $\int_\Delta f(\vec{q},\vec{v})\,d\vec{q}\,d\vec{v}$. In other words, $\mu^{(d)}$ is an approximating sequence if, for each such Δ , the probability (relative to $\mu^{(d)}$) of finding the fraction of particles in Δ nearly equal to $\int_\Delta f(\vec{q},\vec{v})\,d\vec{q}\,d\vec{v}$ goes to one as d goes to zero. (The restriction of the Δ's in this definition to rectangular parallelipipeds (rather than some larger class of subsets) may be puzzling. It would have been equivalent to have replaced "rectangular parallelipiped" by "Borel set whose boundary

has Lebesgue measure zero". Moreover, in the cases we will consider below, we have convergence for all Borel sets Δ. Nevertheless, requiring convergence for all Borel sets would give a much more restrictive definition in general; it would rule out, for instance, approximating sequences in which each $\mu^{(d)}$ is a point mass.) Using this terminology, we can reformulate the basic question as follows: If $\mu^{(d)}$ is an approximating sequence for f, what further conditions are needed in order to guarantee that $\mu^{(d)} T^{-t}$ (μ evolved with the microscopic time development to time t) is an approximating sequence for f_t?

To formulate a set of sufficient conditions we assume first of all:

(0) Each $\mu^{(d)}$ is absolutely continuous with respect to Lebesgue measure, so we can write it as

$$\mu^{(d)}(x_1,\ldots,x_n)dx_1\ldots dx_n$$

(we have abbreviated $(\vec{q}_i,\vec{v}_i)$ to x_i); also $\mu^{(d)}(x_1,\ldots,x_n)$ is a symmetric function of its arguments.

Next we introduce the correlation functions for the measures $\mu^{(d)}$ or more precisely the correlation functions rescaled in a convenient way so that they remain finite in the limit $d \to 0$. Specifically, we define:

$$f_j^{(d)}(x_1,\ldots,x_j) = \frac{n!}{(n-j)!}\frac{1}{n^j}\int dx_{j+1}\ldots dx_n \mu^{(d)}(x_1,\ldots,x_n)$$

(The combinatorial factor $\frac{n!}{(n-j)!}\frac{1}{n^j}$ approaches one as $n \to \infty$ with j fixed, and hence, on a heuristic level should be ignored. It does, nevertheless, play an important role in the estimates, which involve uniformities in n and j.) Most of the useful information about the statistical state $\mu^{(d)}$ is contained in the first few $f_j^{(d)}$'s. In particular for any Borel set Δ,

$$\int d\mu^{(d)} F_\Delta = \int_\Delta f_1^{(d)}(x_1)\,dx_1$$

$$\int d\mu^{(d)} F_\Delta^2 = \int_{\Delta\times\Delta} f_2^{(d)}(x_1,x_2)\,dx_1 dx_2 + \frac{1}{n}\int_\Delta f_1^{(d)}(x_1)\,dx_1$$

From these formulas it is easy to see that $(\mu^{(d)})$ is an approximating sequence for $f_\circ$ if and only if

$$\lim_{d\to 0} f_1^{(d)}(x_1)\,dx_1 = f_\circ(x_1)\,dx_1 \quad \text{and}$$

$$\lim_{d\to 0} f_2^{(d)}(x_1,x_2)\,dx_1 dx_2 = f_\circ(x_1) f_\circ(x_2)\,dx_1 dx_2$$

in the sense of weak* convergence of measures. Moreover, it follows automatically from these conditions that

$$\lim_{d\to 0} f_j^{(d)}(x_1,\ldots,x_j)\,dx_1\ldots dx_j = \prod_{i=1}^{j} f_\circ(x_i)\,dx_i \quad \text{for all } j$$

in the same sense.

We are now able to formulate our main result:

Theorem.

Assume that $f_\circ(\vec{q},\vec{v})$ *is continuous, and let* $\mu^{(d)}$ *be an approximating sequence for* $f_\circ$. *Assume further:*

(1) *There exist constants* $c, \zeta, \beta>0$ *such that*

$$f_j^{(d)}(x_1,\ldots,x_j) \le c\, g_j^{(\zeta,\beta)}(x_1,\ldots,x_j) \quad \textit{for all } d,j,x_1,\ldots,x_j$$

where

$$g_j^{(\zeta,\beta)}(x_1,\ldots,x_j) = \zeta^j \left(\frac{m\beta}{2\pi}\right)^{\frac{3}{2}j} \exp -\frac{\beta m}{2}(\vec{v}_1^{\,2} + \vec{v}_j^{\,2})$$

denote the correlation functions for the non-interacting equilibrium state with density ζ *and inverse temperature* β.

(2) $\lim_{d\to 0} f_j^{(d)}(x_1,\ldots,x_j) = f_\circ(x_1)\ldots f_\circ(x_j)$ *uniformly on compact sets of* $(\Lambda \times \mathbb{R}^3)^j$ *for* j; *by* $(\Lambda \times \mathbb{R}^3)^j$, *we mean* $\{ (\vec{q}_1,\vec{v}_1;\ldots\vec{q}_j;\vec{v}_j) : \vec{q}_i \neq \vec{q}_k \text{ for } i \neq k \}$, *and let* $t_\circ = .2\bar{t} = .2\left(\frac{m\beta}{3}\right)^{\frac{1}{2}}\left(\frac{1}{\pi n d^2}\right)$ *where* β, ζ *are as in* (1). *Then for* $0 \le t \le t_\circ$, $\mu^{(d)}\circ T^{-t}$ *is an approximating sequence for* f_t.

Remarks.

1. The condition (1) may be viewed primarily as a regularity condition on the approximating sequence $\mu^{(d)}$ which prevents building in very strong correlations; it also rules out the presence of a significant number of particles of very high energy which could, in principle, introduce unmanageable perturbations. Note that (1) and (2) together imply

$$f_0(q,v) \leq \mathcal{Z}(\frac{m\beta}{2\pi})^{3/2} \exp -\frac{m\beta}{2} \vec{v}^2$$

2. Condition (2), at least superficially, appears to be a reasonable sort of strengthening of the weak-convergence of $f_j^{(d)}(x_1,\ldots,x_j)dx_1\ldots dx_j$ which is equivalent to the fact that $\mu^{(d)}$ is an approximating sequence for f. We will see shortly, however, that this condition is quite strong (and perhaps unnaturally so).

3. The quantity $\bar{t} = (\frac{m\beta}{3})^{\frac{1}{2}}(\frac{1}{\pi nd^2\mathcal{Z}})$ is the heuristic mean free time for a dilute gas of spheres of diameter d, density n, and inverse temperature β. (In more detail, $(\frac{m\beta}{3})^{-\frac{1}{2}}$ is the r.m.s. velocity and $\frac{1}{\pi nd^2\mathcal{Z}}$ is the mean free path.) Although $\beta, \mathcal{Z}$ are not parameters describing the $\mu^{(d)}$ themselves, but only appear in bounds satisfied by them, we can still expect that, in reasonable cases, $\bar{t}$ will be of the order of magnitude of the mean free time. Our result thus says that the Boltzmann equation describes the correct microscopic motion for a small fraction of a mean free time.

4. Since most of the interesting applications of the Bolzmann equation have to do with the behavior of solutions for large times, it is a serious defect that our results are proved only for short times. While the technique of proof definitely does not extend to larger times, examination of the proof suggests (to me at least) that the result should remain true. One can show, for example, that if the bound (1) holds not only for the initial correlation functions

but also for the time-dependent correlation functions up to time T, and if (2) holds at time zero, then $\mu^{(d)}\ T^{-t}$ is an approximating sequence for f_t up to time $T + t_o$. Thus, it is only the possible failure of bounds which prevent the argument from extending to arbitrarily large times. On the other hand, in order to use the Boltzmann equation to draw conclusions about the large-time behavior of systems of particles of small but finite size, it would be necessary to have not only a theorem like the above for arbitrary times but also some information about uniformity (in time) of convergence; our method of proof gives no indication that there will be any such uniformity. Furthermore, the divergences of the finite-density corrections to the Boltzmann equation make uniformity of convergence problematical. (For a discussion of these divergences, see, for example [3].)

5. For understanding the conceptual problems associated with the Boltzmann equation, on the other hand, our results are less unsatisfactory, as they show that the decrease of Boltzmann's H-function is a consequence of classical mechanics (and the proper choice of initial conditions) and hence that there is no need for external sources of randomness (heat reservoirs, etc.) in order to produce irreversible behavior.

6. We alluded above to difficulties in proving the existence of solutions of the Boltzmann equation, so we must explain how these difficulties relate to our result. We have already noted that the initial f_o satisfies

$$f_o(\vec{q},\vec{v}) \leq \gamma \left(\frac{m\beta}{2\pi}\right)^{3/2} \exp -\frac{m\beta}{2}\vec{v}^2$$

There is a formal series expansion for solutions of the Boltzmann equation obtained by treating the quadratic term as a perturbation on the linear term. This series may be shown to converge for $|t| < t_o$ if f_o satisfies the above bound. This gives an existence

theorem for the interval of times for which our result holds; moreover, the solution obtained is unique in the class of solutions satisfying some mild regularity conditions.

7. We have considered a system in a fixed finite box Λ. This was done only to avoid a further set of complications in the formulation of our results; we could equally well have let Λ become infinitely large as particle size approaches zero. (The condition nd^2 fixed would then be replaced by $\frac{nd^2}{v(\Lambda)}$ fixed.) It would probably even have been possible to have taken Λ and n infinite to start with, although this would have required proving the existence almost everywhere of solutions of the equations of motion for infinitely many hard spheres in a non-equilibrium situation. We emphasize again, however, that we do not get the Boltzmann equation in a simple $n \to \infty$ limit without letting the particle size go to zero. In our view, the Boltzmann equation holds in a regime in which the particle size is very small compared with the mean free path, which in turn is of the same order of magnitude as the distance over which f_0 varies.

It is of interest to examine carefully the effects of the reversibility-irreversibility dichotomy in our theorem. The following argument would appear at first glance to imply that something is wrong: Let $\mu^{(d)}$ be an approximating sequence satisfying (1) and (2), and let t' be some positive number smaller than $t_0/2$. Follow the system to time t' and reverse all velocities. This gives a new approximating sequence, say $\hat{\mu}^{(d)}$, for $f_{t'}(\vec{q},-\vec{v})$. If we follow $\hat{\mu}^{(d)}$ through t' units of time we obtain the original sequence $\hat{\mu}^{(d)}$ with all velocities reversed. On the other hand, the value at time t' of the solution of the Boltzmann equation with initial value $f_{t'}(\vec{q},-\vec{v})$ is definitely not $f_0(\vec{q},-\vec{v})$. A contradiction

would therefore arise if the sequence $\hat{\mu}^{(d)}$, which is indeed an approximating sequence $f_t, (\vec{q},-\vec{v})$, satisfied conditions (1) and (2). Moreover, although condition (1) (presumably) need not hold for $\hat{\mu}^{(d)}$ with the original values of $\mathcal{Z},\beta$, it can be shown to hold for a smaller β' and larger $\mathcal{Z}'$ such that

$$t' < .2\ (\frac{m\beta'}{3})^{1/2}\ \frac{1}{\pi n d^2 \mathcal{Z}'}\ .$$

Thus, the only way to avoid a contradiction is to have (2) fail to hold. Now, in fact, one obtains in the course of proving the theorem quite detailed information about the $\hat{\mu}^{(d)}$, and in particular it turns out that there are surfaces in the j-particle phase space $(j > 1)$ on which the corresponding correlation functions $\hat{f}_j^{(d)}$ do not converge to the desired products of f_t's. Away from these surfaces, locally uniform convergence does occur. One conclusion which can be drawn is that, if condition (2) holds at time zero, it cannot hold at later times. In this sense, (2) is quite a restrictive condition. F. King has shown [2] that the theorem remains valid with (2) replaced by a weaker (but more complicated) condition which does hold at positive times as well as at time zero, but which is not time-reversal invariant.

In introducing our theorem; we indicated that it applies in particular to approximating sequences constructed by an analogue of the microcanonical prescription. There are many different versions of the microcanonical procedure; we will give one of them here. We start as above with:

a. A positive function f_o on $\Lambda \times \mathbb{R}^3$ with unit integral. We will assume that f_o is continuous and also, for simplicity, that it has compact support. Let Σ be some compact set in velocity space $(\mathbb{R}^3)$ such that the support of f_o is contained in $\Lambda \times \Sigma$.

b. A sequence of n's going to infinity and d's going to zero, with nd^2 fixed.

In addition we give:

c. For each d in the sequence, finite partitions $\{\Delta_1^{(d)},\ldots\Delta_{J(d)}^{(d)}\}$ and $\{\Sigma_1^{(d)},\ldots,\Sigma_{K(d)}^{(d)}\}$ of Λ and Σ respectively.

Intuitively, we want the Δ's and Σ's to become arbitrarily small as d approaches zero, but to do so comparatively slowly. We impose these conditions by requiring

d. i. The diameters of the $\Delta_j^{(d)}$ and the $\Sigma_k^{(d)}$ approach zero with d.

ii. The maximum over $j(1 \leq j \leq J(d))$ of the ratio of the volume within a distance d of the boundary of $\Delta_j^{(d)}$ to the volume of $\Delta_j^{(d)}$ itself approaches zero with d.

We also specify, for each d,j,k:

e. an integer $n_{j,k}^{(d)}$ (.the number of particles to be put in the cell $\Delta_j^{(d)} \times \Sigma_k^{(d)}$), subject to the conditions

i. $\lim\inf_{d\to 0} n_{j,k}^{(d)} = \infty$, $\sum_{j,k} n_{j,k}^{(d)} = n$.

ii. $$\lim\sup_{d\to 0} \frac{\left| \frac{n_{j,k}^{(d)}}{n} - \int_{\Delta_j^{(d)} \times \Sigma_k^{(d)}} f(q,v)\,dq\,dv \right|}{\text{volume of } (\Delta_j^{(d)} \times \Sigma_k^{(d)})} = 0$$

In terms of all these objects we construct, for each d, a probability measure $\mu^{(d)}$ by normalizing the restriction of the usual volume in $(\Lambda \times \mathbb{R}^3)^n$ to the set of all phase points satisfying

(*) For each j,k, the number of particles in $\Delta_j^{(d)} \times \Sigma_k^{(d)}$ is equal to $n_{j,k}^{(d)}$

Proposition. The $\mu^{(d)}$'s constructed in this way form an approximating sequence for f which satisfies the hypotheses of the theorem.

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