# ON THE VALIDITY OF THE BOLTZMANN DESCRIPTION AS A CONSEQUENCE OF THE EXACT LAWS OF MECHANICS

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From previous work [2,3] the conditions follow under which a classical spatially nonuniform infinite system obeying the Liouville equation will evolve (irreversibly) according to the Boltzmann integrodifferential equation and satisfy molecular chaos at all times.

It has been made clear in recent years that a basic approach to the study of nonequilibrium phenomena can follow from a close analysis of the laws of microscopic dynamics, for instance trying to relate the Liouville equation to intuitive kinetic equations [1]. A fruitful formal approach in this direction makes use of the projection operator techniques [‡1]. Recently [2], we have proposed along the same lines a new formalism for the analysis of spatially nonuniform fluids in nonequilibrium states which generalizes previous studies on uniform fluids [3–5]. The aim of the present letter is to deepen on the relation between the familiar Boltzmann integrodifferential equation and the Liouville equation as follows from the work in refs. [2] and [3]. In particular we want to state here the conditions of validity of the phenomenological Boltzmann equation, i.e. the precise condition which allows to obtain this equation by "contracting" the description which provides the Liouville equation, and also the validity of the so-called "factorization theorem" in kinetic theory. The gross features of the formalism in ref. [2] are similar to those of uniform fluids [3,4]; so that we only stress here the differences which arise in the case of nonuniform fluids.

We consider a classical conservative system of $N$ identical point-particles of mass $m$ in a volume $V$ whose state at any time $t$ is described by the $N$-body distribution function $F_N$ satisfying the Liouville equation, i.e. $\partial F_N/\partial t = -\mathrm{i}L_N F_N$, where

$$L_N = -\mathrm{i}\sum_{j=1}^{N}\frac{\boldsymbol{p}_j}{m}\cdot\frac{\partial}{\partial \boldsymbol{q}_j} + \mathrm{i}\sum_{j<l}\sum_{l=1}^{N}\frac{\partial\varphi(|\boldsymbol{r}_{jl}|)}{\partial \boldsymbol{q}_j}\cdot\left(\frac{\partial}{\partial \boldsymbol{p}_j}-\frac{\partial}{\partial \boldsymbol{p}_l}\right), \tag{1}$$

$\boldsymbol{r}_{jl} = \boldsymbol{q}_j - \boldsymbol{q}_l$, using familiar notation. The pair potential $\varphi$ corresponds to a repulsive interaction between particles with a finite range $\lambda$. The reduced distribution functions $F_n(q^n, p^n; t)$ corresponding to any set of $n < N$ particles in the system satisfy the well-known BBGKY hierarchy equations. The projection of these equations by means of the projection operator

$$\Gamma\ldots = \frac{1}{V^{n-1}}\int \mathrm{d}q^n\,\delta\left(\frac{1}{n}\sum_{j=1}^{n}\boldsymbol{q}_j - \boldsymbol{R}\right)\ldots\,, \tag{2}$$

where $\delta$ denotes the Dirac delta function and $\boldsymbol{R}$ the position of the center of mass corresponding to the subsystem of $n$ particles, yields in the thermodynamic

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[‡1] See, for instance, ref. [6] and other references quoted therein.

limit ($N \to \infty$, $V \to \infty$, $N/V = D$ finite and constant) a new hierarchy [2] which gives the rate of change of the distribution functions $f_n(\boldsymbol{R}, p^n; t) \equiv \Gamma F_n$. One of the advantages of the equations of this hierarchy is that they only contain, unlike usual series expansions, a finite number of terms at any given order in $D$. The resulting equations are more useful in Fourier space, i.e. when they refer to the time evolution of the Fourier components $\hat{f}_n(\boldsymbol{k}, p^n; t)$, thus obtaining a close similarity between the formalisms for uniform and nonuniform systems.

Let us assume that the above infinite system is in an (initial) state characterized by finite-ranged correlations in the sense that

$$F_n(q^n, p^n; 0) = \prod_{j=1}^{n} F_1(\boldsymbol{q}_j, \boldsymbol{p}_j; 0)[1 + g_n(q^n, p^n; 0)], \tag{3}$$

where the correlation functions $g_n(0)$ vanish if $|\boldsymbol{r}_{jl}| \geqslant \xi$ for all pairs of particles $(j, l)$ (note that $\xi \approx \lambda$). This readily leads in the thermodynamic limit to the factorization of the functions $\hat{f}_n(0)$ in the sense

$$\hat{f}_n(\boldsymbol{k}, p^n; 0) = \prod_{j=1}^{n} \hat{F}_1(\boldsymbol{k}/n, \boldsymbol{p}_j; 0). \tag{4}$$

Moreover, let us assume "small" derivatives with respect to $\boldsymbol{R}$ at $t = 0$, i.e. only weak inhomogeneities in the (initial) state of the system. We may account for this condition in the formalism by introducing a new wave-vector scale $\boldsymbol{k} = D\boldsymbol{\kappa}$ and the limit

$$D \to 0, t \to \infty, Dt = s \text{ finite}. \tag{5}$$

Under the above conditions, the introduction of this limit in the formalism reduces our hierarchy for the rate of change of $\hat{f}_n$ to the form

$$\frac{\partial}{\partial s}\hat{f}_n(\boldsymbol{\kappa}, p^n; s) = -\mathrm{i}\frac{\boldsymbol{P}}{nm}\cdot\boldsymbol{\kappa}\hat{f}_n(\boldsymbol{\kappa}, p^n; s) + \sum_{j=1}^{n} K_{\mathrm{B}}^{(j,n+1)}\hat{f}_{n+1}(\boldsymbol{\kappa}, p^{n+1}; s), \tag{6}$$

where $\boldsymbol{P}$ represents the conjugated momentum of $\boldsymbol{R}$ and $K_{\mathrm{B}}^{(j,n+1)}$ is the Boltzmann collision operator associated with particles $j$ and $n + 1$ [3]. This is accomplished by making an additional assumption which we discuss in the next paragraph. Two features of eq. (6) are to be emphasized. First, the initial correlations (as described by eq. (3)) vanish in the limit (5), thus vanishing the contribution of the initial state in the temporal evolution of $\hat{f}_n(s)$. Second, the wave vector arguments of $\hat{f}_n$ and $\hat{f}_{n+1}$ become identical, i.e. the rate of change of $f_n(\boldsymbol{R})$ depends on sets of $n + 1$ particles with the same center of mass as the original set of $n$ particles. The significance of this point is analyzed at the end of this note.

To obtain eq. (6) we only have to discard from our (exact) hierarchy *one* term which (at finite times) is of order $D^2$. This $D^2$-term, which happens to be the sum of an infinite number of terms in previous perturbative formalisms, contains (in the thermodynamic limit) the dynamics of subsystems of *only two particles* [2,3]. Thus, our method does not deal with an infinite series of terms involving the dynamics of three, four, ..., particles. The $D^2$-term vanishes if a well-defined function of the relative distance of two particles, $r_{jl}$, has a proper limit when $|\boldsymbol{r}_{jl}| \to \infty$ or, equivalently, if the time average of a certain function vanishes. This turns out to be a very reasonable assumption [2,3] and can be proved to be the case for a limited class of potential functions [5].

The conditions stated up to here suffice for a Boltzmann description of the system to be valid in the case of (initial) spatial uniformity, as was previously shown [3] using a projection operator different from (2). In fact, making $\boldsymbol{\kappa} = \boldsymbol{0}$ in eqs. (4) and (6) those equations imply that $f_1(\boldsymbol{p}; s)$ will satisfy the Boltzmann equation (without streaming term) and that $f_n(p^n; s)$ will be factorized as a product of $f_1$'s during the whole system evolution. In the case of nonuniform (actually, weakly nonuniform) systems, however, the system will evolve according to the Boltzmann description when the initial state satisfies molecular chaos in the sense

$$F_n(\boldsymbol{q}, p^n; 0) = \prod_{j=1}^{n} F_1(\boldsymbol{q}, \boldsymbol{p}_j; 0). \tag{7}$$

This completes the conditions which allow to derive in the general case the Boltzmann equation and the persistence of the factorization (7) from the Liouville equation.

We also mention on the significance of conditions (5) and (7) which introduce severe restrictions on the validity of the familiar Boltzmann description. Condi-

tion (5) has been discussed in ref. [6] where it is claimed that, in order to obtain irreversible equations from reversible ones, one needs to introduce a new time scale (concerning our "observations" on the system). The rate of change of $f_n(s)$ (in the new $s$-time scale) is a consequence of many collisions between two instants of observations; the irreversible evolution of the system is thus formally obtained by means of some kind of "temporal coarse-graining". On the other hand, the initial condition (7) is a particular case of the assumption (3). In fact, the probability $F_n(q^n)$ factorizes as a product of $F_1(\boldsymbol{q}_j)$'s for positions such that $|\boldsymbol{r}_{jl}| > \xi$, i.e. if the particles are initially far enough from each other; now for positions $\boldsymbol{q}_j$ such that $|\boldsymbol{r}_{jl}| < \zeta$, where $\zeta$ is the characteristic length for the inhomogeneities in the system (of the order of the inverse of the small gradients $\partial F_n(0)/\partial \boldsymbol{R}$) one can replace every $\boldsymbol{q}_j$ by the same $\boldsymbol{q}$. Thus condition (3) implies (7) when one has $\xi < |\boldsymbol{r}_{jl}| \zeta$ for any pair $(j, l)$ in the given set of $n$ particles. Finally, we note that the identity of the wave vector arguments of $\hat{f}_n$ and $\hat{f}_{n+1}$ in eq. (6) together with the persistence of the molecular chaos in the sense of eq. (7) ($\boldsymbol{q}_j \approx \boldsymbol{q}$) means that the evolution of any set of particles within a small region ($|\boldsymbol{r}_{jl}| < \zeta$) is influenced only by particles in that region.

*References*

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