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On the Time Evolution of the States of Infinitely Extended Particles Systems

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We consider an infinite classical system of interacting particles in $\mathbb{R}^\nu$, $\nu \geqslant 1$. We study the time evolution of a particular class of nonequilibrium states. More precisely, the states we consider are Gibbs with respect to a Hamiltonian which differs from the Hamiltonian governing the motion by an external field (possibly not localized), satisfying certain conditions. It is proved that the time-evolved states satisfy superstable estimate and are described by correlation functions obeying the BBGKY hierarchy in a weak form.

KEY WORDS: Spatial perturbations of equilibrium states; BBGKY hierarchy; time-dependent superstable estimates.

1. INTRODUCTION

The basic problem of nonequilibrium statistical mechanics is the study of the time evolution of the macroscopic states of physical systems. The states are usually defined as probability measures on the phase space of the infinitely extended system,[15] so that one can implement the evolution of the states via the evolution of the phase points, whose existence has to be proved as a first step.

This problem was studied by Lanford in 1968 for classical point particle systems interacting via a two-body bounded, smooth, and short-range potential Φ.[6] He proved an existence and uniqueness theorem for the infinite system of equations:

$$m\dot{q}_i = p_i, \qquad \dot{p}_i = -\sum_{j\neq i} \frac{\partial\Phi}{\partial q_i}(q_i - q_j), \qquad i, j = 1, \ldots, n, \ldots \tag{1.1}$$

for one-dimensional systems and a very large set of initial phase points.

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One can easily see that the problem is highly nontrivial. In fact the set of initial phase points whose evolution is relevant from a thermodynamical point of view must have total infinite energy to be the support of interesting measures. Unfortunately such points may, in principle, develop singular solutions (infinitely many particles in bounded regions or infinite velocities) as in fact some of them do. Thus for this kind of existence theorem, we have to choose with some care the set of initial conditions: large enough for thermodynamical considerations, and small enough to prevent singularities.

The result in Ref. 6 was expanded some years later by Dobrushin and Fritz in two directions: allowing singular potentials[(3)] and two-dimensional systems.[(4)]

These papers are based on one a priori estimate making use of the energy conservation law, that allows crucial cancellations. On the other hand the authors constructed an example which showed that arguments based on the energy conservation law alone can work at most in two dimensions.[(4)] In fact, they proved that very honest initial phase points (having uniformly bounded velocities and densities) may develop singularities in finite time in more than two dimensions. This is discouraging, because it seems difficult to prove that such phase points are negligible for physical reasons. (Reviews on the above may be found in Refs. 7, 8, 13.)

However, there is another approach which, while giving weaker results, works in any dimension (see Refs. 1, 7, 10, 14). This is based on the following idea. Let us consider a Gibbs state μ at some temperature and activity. Such a state is formally invariant with respect to the dynamics given by (1.1), and if we suppose that a μ-nonzero set of initial configurations will develop singularities (e.g., there will be infinitely many particles in a bounded region at some time t), we obtain a contradiction because the probability of finding such singularities is zero with respect to the time-invariant measure μ. The above idea may be used to obtain an existence theorem for the problem (1.1) for a class of initial conditions $\mathcal{X}_0$ such that $\mu(\mathcal{X}_0) = 1$. This set is, however, not explicitly known. Solutions of this kind, but with a somehow detailed qualitative picture of the motion, have been given previously by Sinai.[(17)]

The above solutions (sometimes called equilibrium solutions) apply only to states that are absolutely continuous with respect to the Gibbs state μ, i.e., local perturbations from equilibrium.

All these considerations suggest the study (in dimensions greater than two) directly of the evolution of the states without passing through the evolutions of phase points. This makes sense also from a physical point of view, where the interest lies in the evolution of time-dependent mean values.

In this paper a small step is made in this direction. We investigate the time evolution of an initial state which is Gibbs with respect to a Hamiltonian $H_0 + \tilde{h}$. The time evolution is governed by the Hamiltonian H_0 which consists of both a kinetic and a potential part and $\tilde{h} = \sum h(q_i)$. The external potential $h(q)$ satisfies severe restrictions. For a large class of Hamiltonians H_0 and in any dimension, we prove the existence of a time-evolved state described by a family of correlation functions satisfying the BBGKY hierarchy in a weak form. Moreover, probability estimates, called superstable, are preserved in time (not uniformly). The assumptions on h reduce to the integrability of $(\nabla h)^2$ in the case where h is uniformly bounded. While this does not mean that the state is absolutely continuous with respect to a Gibbs state generated by H_0, nevertheless interesting states, such as Gibbs states with asymptotically different activities, are excluded except in one dimension. On the other hand this analysis improves known results, by considering more general (long-range) potentials and proving strong probability estimates. The case of a localized field (h with compact support) has been previously studied by Gallavotti, Lanford, and Lebowitz in Ref. 5 with methods different from those used in the present paper.

In Section 4, the main results of this work are obtained in a quite straightforward way, following an estimate, deduced in Section 3. Sections 2 and 5 are devoted to definitions and comments.

2. DEFINITIONS AND HYPOTHESES

A system of point particles in a bounded open set Λ, $\Lambda \subset \mathbb{R}^\nu$ is described in the following way. For any bounded set $\Lambda \subset \mathbb{R}^\nu$, let $\mathscr{X}(\Lambda)$ be the grand canonical phase space defined as the symmetrization of

$$\emptyset \cup \left[\bigcup_{n \geqslant 1} (\Lambda \times \mathbb{R}^\nu)^n \right]$$

A point X_Λ in $\mathscr{X}(\Lambda)$ is thus represented by a finite subset of $(\Lambda \times \mathbb{R}^\nu)$. It will be denoted by $X_\Lambda \equiv \{q_1, p_1 \ldots q_n, p_n\}$, n arbitrary, $q_i \in \Lambda$, $p_i \in \mathbb{R}^\nu$, where q_i and p_i denote position and impulsion of the ith particle of the system. $\mathscr{X}(\Lambda)$ is equipped with the usual topology. A state of the system is a Borel probability measure on $\mathscr{X}(\Lambda)$.

Let us introduce also the phase space $\mathscr{X}$ of the infinite system. A point $X \in \mathscr{X}$ is described by a sequence $\{q_i, p_i\}_{i=0}^{\infty}$, $q_i, p_i \in \mathbb{R}^\nu$, with the property that $X \cap (\Lambda \times \mathbb{R}^\nu)$ has finite cardinality for any bounded open set Λ. Two sequences, differing only by a permutation, identify the same point in the phase space $\mathscr{X}$.

Let $f \equiv \{f^n\}_{n \in \mathbb{N}}$ be a sequence of all null, but a finite number, symmetric, continuous functions, $f^n : (\mathbb{R}^\nu \times \mathbb{R}^\nu)^n \to \mathbb{R}$. Assume also that they have compact support. Then a function $\Sigma f : \mathscr{X} \to \mathbb{R}$ may be defined as follows:

$$(\Sigma f)(X) = \sum_{S \subset X} f^{N(S)}(S), \qquad X \in \mathcal{X} \tag{2.1}$$

where the sum in (2.1) is done over all finite subsets S of X and $N(s)$ denotes the cardinality of S. Equation (2.1) makes sense because $\sum_{S \subset X}$ is finite for all $X \in \mathcal{X}$. Furthermore, if all f^n are spatially supported in $\Lambda \subset \mathbb{R}^\nu$, then

$$(\Sigma f)(X) = (\Sigma f)(Y) \qquad \text{if} \quad X \cap (\Lambda^c \times \mathbb{R}^\nu) = Y \cap (\Lambda^c \times \mathbb{R}^\nu) \tag{2.2}$$

The set of all Σf's will be denoted by $\mathcal{A}$. $\mathcal{A}$ is an algebra. $\mathcal{X}$ will be thought of as a topological space with a topology which is the minimal one, making continuous all the functions of $\mathcal{A}$. With this topology $\mathcal{X}$ is complete, metrizable, and separable. In the sequel we will find useful the subset of $\mathcal{A}$, denoted by $\mathcal{A}^n$, of all functions generated by a single n-body function—i.e.,

$$\mathcal{A}^n \equiv \left\{ \Sigma f \,|\, (\Sigma f)(X) = \sum_{\substack{S \subset X \\ N(S)=n}} f^n(S) \right\} \tag{2.3}$$

We define also, in a complete analogous way, the subalgebra $\mathcal{A}_\infty$ and the subset $\mathcal{A}^n_\infty$ of $\mathcal{A}$, as the family of all functions $\Sigma f \in \mathcal{A}$ generated by infinite differentiable functions f^n.

A state of the infinite-particle system is described by a Borel probability measure on $\mathcal{X}$.

Given a state ν on $\mathcal{X}$, the family of correlation functions $\{\rho_n^\nu\}$ associated to ν (if it exists) is defined by the following relations:

$$\int \rho_n^\nu(x_1 \ldots x_n) f^n(x_1 \ldots x_n) \frac{dx_1 \ldots dx_n}{n!} = \int \nu(dX)(\Sigma f)(X) \tag{2.4}$$

for $\Sigma f \in \mathcal{A}^n$, $X_i = (q_i, p_i)$.

Among the class of states, the so-called Gibbs states have particular relevance. They are defined as follows. For any bounded open set $\Lambda \subset \mathbb{R}^\nu$, let $H : \mathcal{X}(\Lambda) \to \mathbb{R}$ a family of measurable functions. Then for any $X \in \mathcal{X}$, define the following probability Borel measure on $\mathcal{X}(\Lambda)$:

$$P(dY_\Lambda \,|\, X_\Lambda c) = \frac{\lambda(dY_\Lambda)}{Z_\Lambda(X_\Lambda c)} \exp\{-H(Y_\Lambda) - H(Y_\Lambda \,|\, X_\Lambda c)\} \tag{2.5}$$

where

$$X_\Gamma = X \cap (\Gamma \times \mathbb{R}^\nu), \quad \Gamma \subseteq \mathbb{R}^\nu, \quad Y_\Lambda \in \mathcal{X}(\Lambda) \tag{2.6}$$

$$H(Y_\Lambda \,|\, X_\Lambda c) = \lim_{\Omega \nearrow \Lambda^c} \{H(Y_\Lambda \cup X_\Omega) - H(Y_\Lambda) - H(X_\Omega)\} \tag{2.7}$$

and the above limit is taken over a family of increasing bounded sets Ω

invading Λ^c,

$$\lambda(dY_\Lambda) = 1 + \sum_{n=1}^{\infty} \frac{dq_1 \ldots dq_n dp_1 \ldots dp_n}{n!} \tag{2.8}$$

and finally, $Z_\Lambda(X_{\Lambda}c)$ is a normalization factor. Then a Gibbs state with respect to the family of Hamiltonians $\{H\}$ is any probability measure μ on $\mathscr{X}$ satisfying the equations

$$\int \mu(dX) f(X) = \int \mu(dX) \int P(dX_\Lambda \mid X_{\Lambda}c) f(Y_\Lambda \cup X_{\Lambda}c) \tag{2.9}$$

where f is a bounded continuous function, provided that the limit (2.7) exists at least for μ almost all $X \in \mathscr{X}$.

Solutions of Eqs. (2.9) (called the DLR equations after the works of Dobrushin, Lanford, and Ruelle[2,9]) may be proven to exist, in many cases of interest for the classical statistical mechanics of one-component systems, where

$$H(X_\Lambda) = \beta T(X_\Lambda) + \beta V(X_\Lambda) + \beta\bar{\mu} N(X_\Lambda) \tag{2.10}$$

$$T(X_\Lambda) = \frac{1}{2m} \sum_{i=1}^{N(X_\Lambda)} P_i^2 \qquad (m \text{ is the mass of particles}) \tag{2.11}$$

$$V(X_\Lambda) = V(q_1, \ldots, q_{N(X_\Lambda)}), \qquad V: \Lambda^n \to \mathbb{R} \quad \text{symmetric} \tag{2.12}$$

and $\beta > 0$ and $\bar{\mu} \in \mathbb{R}$ are the two macroscopic parameters, the inverse temperature and the chemical potential, describing the thermodynamic equilibrium.

It may be proven,[16] that sufficient conditions for the existence of Gibbs measures of such type are (Λ open, bounded)

$$V(X_\Lambda) \geqslant A \frac{N(X_\Lambda)^2}{|\Lambda|} - BN(X_\Lambda) \qquad \text{for some} \quad A, B > 0 \tag{2.13}$$

here $|\Lambda|$ denotes the volume of Λ.

Moreover, given a covering $\mathscr{Q}$ of $\mathbb{R}^\nu$ in terms of elementary cubes of fixed side, denoted by Δ, Δ' etc., there exists a positive decreasing function $\bar{\varphi}$ such that

$$\sum_{\Delta' \in \mathscr{Q}} \bar{\varphi}(d(\Delta', \Delta)) < +\infty \tag{2.14a}$$

$$H(X_\Lambda \mid Y_{\Lambda}c) \geqslant - \sum_{\Delta \in 2} \sum_{\substack{\Delta' \in \mathscr{Q} \\ \Delta' \neq \Delta}} \bar{\varphi}(d(\Delta', \Delta)) \{ N_\Delta^2(X_\Lambda) + N_{\Delta'}^2(Y_{\Lambda}c) \} \tag{2.14b}$$

where $d(\Delta', \Delta)$ is the Euclidean distance between the centers of the cubes Δ', Δ. Here and after N_Ω denotes the function number of particles in the region Ω.

Properties (2.13) and (2.14) are called, respectively, superstability and lower regularity.

We want to study the time evolution of a Gibbs state μ generated by a family H of Hamiltonians (2.10), in which

$$V(X_\Lambda) = V_0(X_\Lambda) + \tilde{h}(X_\Lambda) \tag{2.15}$$

under the action of the dynamics generated by

$$H_0(X_\Lambda) = T(X_\Lambda) + V_0(X_\Lambda) \tag{2.16}$$

We assume (although not strictly necessary) V_0 to be a potential energy generated by a single two-body potential $\Phi : (0, +\infty) \to \mathbb{R}$, i.e.,

$$V_0(q_1 \ldots q_n) = \frac{1}{2} \sum_{i \neq j} \Phi(|q_i - q_j|) \tag{2.17}$$

Φ continuously differentiable and such that (2.13) and (2.14) hold (with V replaced by V_0). We further require

$$|\Phi'(r)| \leqslant \Phi(r)^\delta + G \qquad \text{for some} \quad G > 0, \quad \delta > 1 \tag{2.18}$$

and

$$\sum_{\substack{\Delta' \in \mathcal{D} \\ \partial\Delta' \cap \partial\Delta = \emptyset}} F(\Delta, \Delta') = F < +\infty \tag{2.19}$$

where

$$F(\Delta, \Delta') = \sup_{\substack{x \in \Delta \\ x' \in \Delta'}} \left| \frac{\partial \Phi(|x - x'|)}{\partial x} \right| \tag{2.20}$$

It is easily seen that all honest two-body interactions, possibly diverging at the origin, and with integrable long range, satisfy the above requirement.

$\tilde{h}$ is assumed to be of the form

$$\tilde{h}(X_\Lambda) = \sum_{\substack{i: \\ q_i \in X_\Lambda}} h(q_i) \tag{2.21}$$

where $h : \mathbb{R}^\nu \to \mathbb{R}$ is a positive, continuously differentiable function satisfying the following condition:

$$\int e^{-h(q)} \left[\exp\left(\frac{\partial h}{\partial q} \right)^2 - 1 \right] dq < +\infty \tag{2.22}$$

Although condition (2.22) is too restrictive to cover all physically interesting cases of spatial perturbations (especially for $\nu > 1$), it does not imply the absolute continuity of the state μ with respect to some Gibbs state generated by H_0, since (2.21) may hold, without h being integrable. The existence of solutions of the DLR equations follows, in our case, by the following estimate.[16]

Let μ_Λ be a finite-volume Gibbs state with respect to a family of Hamiltonians (2.10) satisfying (2.15) with V_0 superstable and lower regular and h continuous and positive. Let $\{\rho_\Lambda\}$ be the family of correlation functions associated to μ_Λ. Then there exist positive numbers λ and ξ, not depending on Λ, such that for any $\Omega \subset \Lambda \subset \mathbb{R}^\nu$, Ω measurable, the following estimate holds:

$$\rho_\Lambda(X_1 \ldots X_n) \leqslant \xi^n \exp\left\{ -\frac{\lambda n^2}{|\Omega|} - \beta\left[\sum_{i=1}^{n} h(q_i) + \frac{p_i^2}{2m} \right]\right\} \tag{2.23}$$

where

$$X_i = (q_i, p_i), \qquad q_i \in \Omega$$

A probabilistic consequence of (2.23) is that the μ_Λ probability of finding more than n particles in Ω is bounded by

$$\exp\left[-(K_1/|\Omega|)n^2 + K_2 n \right] \tag{2.24}$$

for some K_1 and K_2 not depending on Λ.

We refer to (2.24) as the superstable estimates. They allow the construction of a compact set on $\mathcal{X}$ in which the measures $\{\mu_\Lambda\}$ are almost concentrated, and thus the existence (by compactness) of limiting measures μ satisfying the DLR equations together with the superstability estimates. Moreover any limiting state is described by correlation functions satisfying (2.23).

3. BASIC ESTIMATE

The main idea of this section is the following. Suppose the existence of the Hamiltonian dynamics generated by H_0 as a μ almost everywhere defined measurable flow $\tilde{\gamma}_t$ on $\mathcal{X}$.

Let us denote by γ_t its action on the functions

$$(\gamma_t f)(x) = f(\tilde{\gamma}_{-t}x), \qquad x \in \mathcal{X}, \qquad t \in \mathbb{R}, \qquad f \in L_p(\mathcal{X}, \mu), \qquad p > 1 \tag{3.1}$$

Then γ_t has the formal generator $\{., H_0\}$, where $\{.,.\}$ denotes the Poisson brackets. Then obviously

$$\{., H_0\} = \{., H_1\} - \{., \tilde{h}\} \tag{3.2}$$

where $H_1 = H_0 + \tilde{h}$. Now the flow generated by $\{., H_1\}$ is already proved to exist (equilibrium dynamics) and leaves μ invariant, while the flow generated by $\{., h\}$ is very simple: all particles are frozen and vary their momenta accordingly to the field h. So one can hope to control the finite-volume dynamics generated by $\{.,H_0\}$, combining these two facts. With this in mind, we denote by Λ a ν-dimensional open sphere centered at the origin with arbitrary radius. For a fixed $x \in \mathfrak{X}$, we are looking for trajectories in $\mathfrak{X}$ satisfying

$$\left.\begin{aligned} \dot{q}_i^{\Lambda}(t) &= \frac{\partial H_0(X_\Lambda(t))}{\partial p_i} \\ \dot{P}_i(t) &= -\left(\frac{\partial H_0(X_\Lambda(t))}{\partial q_i} + \frac{\partial H_0\left(X^{\Lambda}(t)\,|\,X^{\Lambda^c}\right)}{\partial q_i}\right) \end{aligned}\right\} \quad \text{if} \quad q_i(0) = q_i \in \Lambda$$

$$\left.\begin{aligned} \dot{q}_i(t) &= 0 \\ \dot{p}_i(t) &= 0 \end{aligned}\right\} \quad \text{if} \quad q_i \in \Lambda^c \tag{3.3}$$

$$X_\Lambda(0) \equiv X_\Lambda = X \cap (\Lambda \cap \mathbb{R}^\nu), \qquad X = \{q_i, P_i\}_{i=1}^{\infty}$$
$$X_\Lambda c = X \cap (\Lambda^c \cap \mathbb{R}^\nu), \qquad \text{initial conditions}$$
elastic collision in $\partial\Lambda$

$$\left.\begin{aligned} \dot{q}_i^{\Lambda}(t) &= \frac{\partial H_1(X_\Lambda(t))}{\partial p_i} \\ \dot{p}_i^{\Lambda}(t) &= -\left[\frac{\partial H_1(X_\Lambda(t))}{\partial q_i} + \frac{\partial H_1(X_\Lambda(t)\,|\,X_\Lambda c)}{\partial q_i}\right] \end{aligned}\right\} \quad \text{if} \quad q_i(0) = q_i \in \Lambda$$

$$\left.\begin{aligned} \dot{q}_i^{\Lambda}(t) &= 0 \\ \dot{p}_i^{\Lambda}(t) &= 0 \end{aligned}\right\} \quad \text{if} \quad q_i \in \Lambda^c \tag{3.4}$$

same initial and boundary conditions as above

$$\begin{aligned} \dot{q}_i^{\Lambda}(t) &= 0 \\ \dot{p}_i^{\Lambda}(t) &= \frac{\partial \tilde{h}}{\partial q_i}, \qquad \text{if} \quad q_i \in \Lambda \\ \dot{p}_i^{\Lambda}(t) &= 0, \qquad \text{if} \quad q_i \notin \Lambda \end{aligned} \tag{3.5}$$
same initial conditions

Let us denote by $\tilde{\gamma}^{\Lambda}$, $\tilde{\alpha}^{\Lambda}$, $\tilde{\beta}^{\Lambda}$ the one-parameter measurable flows satisfying the evolution problems (3.3), (3.5). In constructing $\tilde{\gamma}^{\Lambda}$ and $\tilde{\alpha}^{\Lambda}$ some problems may arise. Firstly, the time independent field $\partial H_k(.\,|\,X_\Lambda c) /\partial q_i$, $k = 0, 1$ may be singular for some $x \in \mathfrak{X}$. But with our assumptions, this is not the case for μ almost all $x \in \mathfrak{X}$.

Secondly, if one starts with a local solution [in all the case in which with μ probability one $(\partial H_k/\partial q_i)(.\,|\,X_\Lambda c)$ is not singular] up to the time of the first collision, and then tries to obtain a global solution with the aid of the elastic reflection law, one cannot a priori exclude the possibility of tangent collisions and that a particle can suffer infinitely many hits with the boundary, in a finite interval of time. In Ref. 11 it is proved that these pathologies can occur at most for a set N of initial configuration X_Λ of λ-measure 0. This allows us to define $\tilde{\gamma}^\Lambda$ and $\tilde{\alpha}^\Lambda$ as measurable flow on $(\mathfrak{X}, \mu)$ and this is enough for our purpose.

Denoting by γ_t^Λ, α_t^Λ, β_t^Λ, the action of the above flows on the functions following definition (3.1), the following hold

$$\|\alpha_t^\Lambda f\|_p = \|f\|_p, \qquad f \in L_p(\mathfrak{X}, \mu), \qquad P \geqslant 1 \tag{3.6}$$

$$\|\beta_t^\Lambda f\|_p^p \leqslant \int \mu(dx)\, e^{A_\Lambda t} |f(X)|^p \tag{3.7}$$

where $\|\cdot\|_p$ denotes the L_p norm with respect to μ, and

$$A_\Lambda(X) = -2\beta \sum_{\substack{i: \\ q_i \in \Lambda}} \left[p_i \cdot \frac{\partial h}{\partial q_i}(X) \right], \qquad X \in \mathfrak{X} \tag{3.8}$$

Equation (3.6) follows by the DLR equations, the Liouville theorem, and energy and particle number conservations.

Proof of (3.7). By the DLR equations, the right-hand side of (3.7) is $(z = \exp - \beta\mu)$

$$\int \mu(dX) \frac{1}{Z_\Lambda(X_\Lambda c)} \sum_{n \geqslant 0} \frac{z^n}{n!} \int_{(\Lambda \times \mathbb{R}^\nu)^n} dq_1 \ldots dq_n\, dp_1 \ldots dp_n$$
$$\times |f(q_1 \cdots q_n\, p_1 \cdots p_n \cup X_\Lambda c)|^p$$
$$\times \exp\left\{ -\beta \left[\sum_{i=1}^n \tilde{\beta}^\Lambda_{-t}(p_i)^2 - V(q_1 \ldots q_n) - H_1(q_1 \ldots q_n | X_\Lambda c) \right] \right\} \tag{3.9}$$

because the Jacobian of transformation $\tilde{\beta}_t^\Lambda$ is one and

$$\tilde{\beta}^\Lambda_{-t}(p_i) = p_i - t \frac{\partial h}{\partial q_i} \tag{3.10}$$

So estimate (3.8) follows by neglecting $t^2(\partial h/\partial q_i)^2$ by positivity.

Let us define

$$g(X) = \Sigma \left(\frac{\partial h}{\partial q} \right)^2 \tag{3.11}$$

As a consequence of our assumptions, $\exp g \in L_p(\mathfrak{X}, \mu)$, $p \geqslant 1$.

In fact the n-body correlation functions of μ are bounded by

$$\prod_{i=1}^{n}\left\{\exp\left[-\beta p_i^2-\beta h(q_i)\right]\right\}\cdot\xi \tag{3.12}$$

that are exactly the correlations functions associated to a Gibbs state of free particles with chemical potential $\log\xi/\beta$ and with an external field h. Let us call such Gibbs state ν. Then $\int\exp(p\cdot g)(x)\,d\mu\leqslant\int\exp(p\cdot g)(x)\,d\nu$ and the latter integral may be computed explicitly. An easy calculation shows that it converges if and only if condition (2.22) is satisfied. The next one is an estimate uniform in Λ that will allow us to get all results concerning the existence and properties of the infinite-volume time-evolved state.

Proposition 3.1. For any measurable $f:\mathfrak{X}\to\mathbb{R}$ and any real positive even function φ the following estimate holds:

$$\|\gamma_t^\Lambda f\|_1\leqslant\left[\int\left\{\exp\left[\beta\left(\frac{t}{\varphi(t)}\right)^2 g\right]\right\}d\mu\right]\|f\|_{\exp\varphi(t)} \tag{3.13}$$

provided the right-hand side of (3.13) makes sense.

Proof. By the use of the Trotter formula

$$\gamma_t^\Lambda f=\lim_{n\to+\infty}\left(\beta_{t/n}^\Lambda\alpha_{t/n}^\Lambda\right)^n f \tag{3.14}$$

where the above limit is taken μ-almost everywhere. Putting $\delta_t^\Lambda=\beta_t^\Lambda\alpha_t^\Lambda$, we want to estimate $(\delta_{t/n}^\Lambda)^n f$ uniformly in Λ and n.

As a consequence of the Hölder inequality and (3.7)

$$\|\beta_t^\Lambda f\|_p\leqslant\|f\|_{pr}\|e^{A_\Lambda t}\|_s^{1/p} \tag{3.15}$$

$p\geqslant 1$ and r and s conjugate exponents. Hence

$$\begin{aligned}\left\|\left(\delta_{t/n}^\Lambda\right)^n f\right\|_1&=\left\|\beta_{t/n}^\Lambda\alpha_{t/n}^\Lambda\left(\delta_{t/n}^\Lambda\right)^{n-1}f_1\right\|\leqslant\|e^{A_\Lambda t/n}\|_s\left\|\alpha_{t/n}\left(\delta_{t/n}^\Lambda\right)^{n-1}f\right\|_r\\&\leqslant\|e^{A_\Lambda t/n}\|_s\left\|\left(\delta_{t/n}^\Lambda\right)^{n-1}f\right\|_r\leqslant\cdots\\&\leqslant\|e^{A_\Lambda t/n}\|_s^{\sum_{k=0}^{n-1}(1/r)^k}\|f\|_{r^n}\end{aligned} \tag{3.16}$$

where we have used (3.15) and the isometric nature of $\alpha_{t/n}^\Lambda$, (3.6).

By the use of DLR equations, and performing the Gaussian integrations on the momenta

$$\int\exp\left(\frac{st}{n}A_\Lambda\right)d\mu=\int\exp\left[\beta\left(\frac{ts}{n}\right)^2\sum_{\substack{i:\\q_i\in\Lambda}}\left(\frac{\partial h}{\partial q_i}\right)^2\right]d\mu\leqslant\int\exp\left[\beta\left(\frac{ts}{n}\right)^2 g\right]d\mu \tag{3.17}$$

Moreover

$$\frac{1}{s}\sum_{k=0}^{n-1}\left(\frac{1}{r}\right)^k = 1 - \frac{1}{r^n} \tag{3.18}$$

putting

$$r = \left[1 + \frac{\varphi(t)}{n}\right] \qquad \text{and hence} \quad s = \left[\frac{n}{\varphi(t)} + 1\right] \tag{3.19}$$

Thus:

$$\left\|(\delta^{\Lambda}_{t/n})^n f\right\|_1 \leqslant \left(\int \exp\left\{\beta g\left[\frac{t}{\varphi(t)} + \frac{t}{n}\right]^2\right\} d\mu\right)^{1-\exp[-\varphi(t)]} \|f\| \exp \varphi(t) \tag{3.20}$$

and the thesis follows by standard arguments.

Let us interpret Proposition 3.1 compared with condition (2.22). Let us put $f = N_\Omega$. Proposition 3.1 says that the time-evolved expectation value of N_Ω remains bounded for each time, as Λ increases, provided (2.22) is satisfied. There are two cases. If h is asymptotically divergent the particles gas is asymptotically rarefied, thus, also if the gradient is increasing, the low density prevents singularities. If h is bounded, the gradient must vanish asymptotically, so that it cannot perturb the equilibrium motion in a singular way.

4. THE EVOLUTION OF THE STATES

Let Σ_n be the ν-dimensional open sphere of center 0 and radius n, with n a positive integer, and $\gamma_t^n = \gamma_t^{\Sigma_n}$.

A natural question arises. If we denote by $\gamma_t^n\mu$ the evolution of the state μ under the action of γ_t^n, i.e.,

$$(\gamma_t^n\mu)(A) = \mu(\gamma_{-t}^n\chi_A) \tag{4.1}$$

$A \subset \mathfrak{X}$ is a Borel set and χ_A is the indicator function of A, then one could define the evolved state $\gamma_t\mu$, under the action of the infinite dynamics, as the weak limit of $\gamma_t^n\mu$, provided such a limit exists.

It is possible to prove the existence of such a limit, for subsequence, closely following standard arguments of equilibrium statistical mechanics of noncompact systems. In fact, by virtue of Proposition 3.1, putting $f = \exp[\zeta(t)N_\Omega^2]/|\Omega|$, where $\zeta(t) = \zeta e^{-|t|}$, and $\zeta > 0$ sufficiently small, then

$$\int (\gamma_t^n\mu)(dX)\exp\left[\zeta(t)\frac{N^2_{\Omega(x)}}{|\Omega|}\right] \leqslant \left\{\int \mu(dx)\exp\left[\zeta\frac{N^2_{\Omega(x)}}{|\Omega|}\right]\right\}^{e^{-|t|}} C_3 \tag{4.2}$$

(where $C_3 = \int \beta e^g \, d\mu$) after choosing $\varphi(t) = |t|$ for the sake of concreteness.

Superstable estimates (2.24) over the initial state μ and the Tchébychev inequality allow us to prove superstable estimates also for the time-evolved states $\gamma_t^n\mu$ (uniformly in n). Thus for any fixed time t we define, by compactness, $\gamma_t\mu$ as a weak limit.

We now prove the following statement:

If for fixed t, $\gamma_t^{n_k}\mu$ converges weakly to a measure $\gamma_t\mu$ for $k \to +\infty$, then $\lim_{k\to+\infty}(\gamma_t^{n_k}\mu)(\Sigma f) = \gamma_t\mu(\Sigma f)$ for all $\Sigma f \in \mathcal{Q}$. (Recall that $\mathcal{Q}$ is an algebra of unbounded functions.)

In fact

$$\begin{aligned}\int(\gamma_t^n\mu)(dx)|\Sigma f(x)| &\leqslant \sum_{n\geqslant 0}\int(\gamma_t^n\mu)(dx)\sum_{\substack{S\subset X\\ N(s)=h}}|f^h(s)|\\ &\leqslant \sup_h \|f^h\|_\infty C_4\int(\gamma_t\mu)(dx)\,N_\Omega(x)^\alpha \qquad (4.3)\end{aligned}$$

where Ω is a spatial support for all the $f^{(n)}$'s and C_4 and α are positive constants depending only on the number, different from zero, of f^h generating Σf. Thus $\mathcal{Q} \in L_p(\mathfrak{X}, \gamma_t\mu)$.

Moreover if

$$\varphi_M(r) = \begin{cases} r & \text{for } -M \leqslant r \leqslant M \\ M & \text{otherwise}\end{cases} \qquad (4.4)$$

$$\begin{aligned}(\gamma_t^n\mu)\left[\Sigma f - \varphi_M(\Sigma f)\right] &\leqslant 2(\gamma_t^n\mu)\left[|\Sigma f|\chi(|\Sigma f| \geqslant M)\right]\\ &\leqslant 2(\gamma_t^n\mu)(|\Sigma f|^2)^{1/2}(\gamma_t^n\mu)\left[\chi(|\Sigma f| \leqslant M)\right]^{1/2}\\ &\leqslant 2\frac{D(f,t)}{\sqrt{M}} \qquad (4.5)\end{aligned}$$

where $\chi(|\Sigma f| \geqslant M)$ is the indicator of the set $\{\Sigma f > M\}$ and $D(f,t)$ is a positive constant depending only on f and t.

The estimate (4.5) combined with an $\epsilon/3$ argument proves the statement.

We now prove the existence of a common subsequence of integers, n_i, such that, for all $t \in \mathbb{R}$,

$$\lim_{i\to\infty}(\gamma_t^{n_i}\mu)(\Sigma f) = (\gamma_t\mu)(\Sigma f), \qquad \Sigma f \in \mathcal{Q}_\infty \qquad (4.6)$$

and the above convergence is uniform in t on compact sets. To this purpose, it is enough to prove the equicontinuity of the family $(\gamma_t^n\mu)(\Sigma f)$ for fixed Σf, and combine it with the usual diagonal trick. The equicontinuity follows easily by recognizing that, for sufficiently large n the following identity holds:

$$\frac{d}{dt}(\gamma_t^n\mu)(\Sigma f) = (\gamma_t^n\mu)(\mathfrak{L}\Sigma f) \tag{4.7}$$

where

$$\mathfrak{L}\Sigma f = \sum_i \left(\frac{\partial \Sigma f}{\partial q_i} \cdot P_i - \frac{\partial \Sigma f}{\partial p_i} \cdot \frac{\partial V_0}{\partial q_i} \right) \tag{4.8}$$

So it is enough to prove the boundness of $(\gamma_t^n\mu)(\mathfrak{L}\Sigma f)$ uniformly in n and t on compact sets. The first term on the right-hand side of (4.8) does not create problems, since it belongs to $\mathcal{C}$, so (4.2) and (4.3) may be used. The second one is bounded by

$$C_5 N_\Omega(x)^\alpha \left| \sum_{\substack{i: \\ q_i \in \Omega}} F_i(x) \right| \tag{4.9}$$

where $C_5 > 0$ depends only on f,

$$F_i(x) = -\sum_{j \neq i} \frac{\partial \Phi(q_i - q_j)}{\partial q_i}$$

and Ω is a spatial support for Σf. Moreover, (4.9) may be bounded by:

$$C_5 N_\Omega(X)^\alpha \left\{ \left[\left[\sum_{\substack{i,j: \\ q_i, q_j \in \Omega}} |\Phi(q_i - q_j)|^\delta \right] + G N_{\bar{\Omega}}^2(x) \right\} \right.$$

$$\left. + \sum_{\substack{\Delta: \\ \Delta' \cap \Omega \neq \varnothing}} \sum_{\substack{\Delta': \\ \Delta' \cap \partial\Delta = \varnothing}} N_\Delta N_{\Delta'} F(\Delta, \Delta') \right] \tag{4.10}$$

where $\bar{\Omega} \supset \Omega$ is a suitably chosen bounded region.

Thus Proposition 3.1, (2.19) and superstable estimates on the initial state μ, allow us to obtain a n-independent bound on the expectation value of (4.10) with respect to $(\gamma_t^n\mu)$.

The same argument used above allows us also to prove that $\mathfrak{L}\Sigma f \in Lp(\mathcal{X}, \gamma_t\mu)$, $p \geqslant 1$ and

$$\lim_{i \to +\infty} (\gamma_t^{n_i}\mu)(\mathfrak{L}\Sigma f) = (\gamma_t\mu)(\mathfrak{L}\Sigma f) \tag{4.11}$$

We may summarize all the results obtained in the following form.

Theorem 4.1. There exists a one-parameter group of probability Borel measure on $\mathcal{X}$, $\{\gamma_t\mu\}_{t\in\mathbb{R}}$ and a subsequence $\{n_i\}$ of positive integers such that

(i) $$\lim_{i\to+\infty}(\gamma_t^{n_i}\mu)(\Sigma f)=(\gamma_t\mu)(\Sigma f),\qquad \Sigma f\in\mathcal{Q} \tag{4.12}$$

(ii) $\gamma_t\mu$ satisfy the superstable estimate for any $t\in\mathbb{R}$ and hence $\mathcal{Q}\in L_p(\mathcal{X},\gamma_t\mu)$, $p\geqslant 1$.

(iii) For any $\Sigma f\in\mathcal{Q}_\infty$, $(\gamma_t\mu)(\Sigma f)$ is differentiable in t and satisfies

$$\frac{d}{dt}(\gamma_t\mu)(\Sigma f)=(\gamma_t\mu)(\mathcal{L}\Sigma f) \tag{4.13}$$

The above result may be read in terms of correlation functions as follows. The estimate (4.3)

$$\int(\gamma_t\mu)(\Sigma f)\leqslant \cos t\|f^{(n)}\|_\infty,\qquad \Sigma f\in\mathcal{Q}_n \tag{4.14}$$

combined with the Riesz theorem, imply the existence of a family of symmetric, σ-finite (unnormalized) measure $d\rho_n^t$ on $(\mathbb{R}^\nu\times\mathbb{R}^\nu)^n$ such that, for all $t\in\mathbb{R}$,

$$\int(\gamma_t\mu)(\Sigma f)=\int\frac{d\rho_n^t}{n!}f^n(x_1\ldots x_n) \tag{4.15}$$

Moreover, if A is a bounded set of Lebesgue null measure, from the equality

$$\int_A\frac{d\rho_t^n(x_1\ldots x_n)}{n!}=(\gamma_t\mu)(\Sigma\chi_A) \tag{4.16}$$

(where $\Sigma\chi_A$ is defined in an obvious way), Proposition 3.1, and the continuity of initial state correlations functions, there follows the absolute continuity with respect to the Lebesgue measures of the measures $d\rho_t^n$. Thus (4.13) may be written, by straightforward computations:

$$\frac{d}{dt}\rho_t(f)=\rho_t(\mathcal{L}_0 f)-\rho_t(f_1),\qquad f\in C_0^\infty(\mathbb{R}^\nu\times\mathbb{R}^\nu)^n \tag{4.17}$$

where

$$\rho_t(f)=\int dx_1\ldots dx_n\,\rho_n^t(x_1\ldots x_n)f(x_1\ldots x_n) \tag{4.18}$$

and ρ_t^n are the densities of the measure $d\rho_t^n$.

$$(\mathcal{L}_0 f)(x_1\ldots x_n)=\sum_{i=1}^n\left(\frac{\partial H_0}{\partial p_i}\frac{\partial f}{\partial q_i}-\frac{\partial H_0}{\partial q_i}\frac{\partial f}{\partial p_i}\right) \tag{4.19}$$

$$f_1(x_1\ldots x_n,x_{n+1})=\sum_{i=1}^n\frac{\partial\Phi}{\partial q_i}(q_i-q_{n+1})\frac{\partial f}{\partial p_i} \tag{4.20}$$

The equations (4.17) are called BBGKY hierarchy. To summarize, we state the following theorem.

Theorem 4.2. The evolved measure $\gamma_t \mu$ are described by correlation functions that satisfy the BBGKY hierarchy in the weak form given by (4.17).

5. CONCLUDING REMARKS

The results of the previous sections may be improved by the use of some arguments of the equilibrium dynamics. Since such arguments are already known and it needs slight modifications in our nonequilibrium context, the proof of the statements of this section will be only sketched.

Define:

$$\varphi(x) = \max(\log x, 1), \qquad x > 0 \tag{5.1}$$

$$G(X) = \sup_{\mu} \sup_{\sigma > \varphi \subset \mu} \frac{G_{\mu,\sigma}(X)}{\sigma^{\nu}} \tag{5.2}$$

$$G_{\mu,\sigma}(X) = \sum_{i}{}_{\mu,\sigma} \left[\frac{p_i^2}{2m} + \frac{1}{2} \sum_{j \neq i}{}_{\mu,\sigma} \Phi(|q_i - q_j|) + B \right] \tag{5.3}$$

where $\sum_{\mu,\sigma}$ means that the sum is restricted to those particles that are in the spherical open region with center μ and radius σ. $G_{\mu,\sigma} > 0$ if B is large enough. It is not hard to see that G is $L_p(\mu)$, $p > 1$ and that the set $\{G < +\infty\}$ is full with respect to μ. Moreover

$$\int \mu(dx)\, G(\gamma_t^{\Lambda} x) \leqslant h(t) \| G \|_e \tag{5.4}$$

by Proposition 3.1, where $h > 1$ is an increasing function. Define

$$\int_{-\infty}^{+\infty} dt\, \frac{e^{-|t|}}{h(t)}\, G(\gamma_t^{\Lambda} x) = \tilde{G}_{\Lambda}(x) \tag{5.5}$$

$$\tilde{G}_{\infty}(X) = \liminf_{\Lambda \to \mathbb{R}^{\nu}} \tilde{G}_{\Lambda}(x) \tag{5.6}$$

As a consequence of Fatou's lemma, the Fubini theorem, and (5.4)

$$\int \mu(dx)\, \tilde{G}_{\infty}(x) \leqslant 4 \| G \|_e \tag{5.7}$$

Thus $\tilde{G}_{\infty}$ is μ-almost everywhere finite, and for μ almost all $X \in \mathfrak{X}$, there can be found a sequence $\Lambda \nearrow \mathbb{R}^{\nu}$ such that $\tilde{G}_{\Lambda}(X) \leqslant C(X)$, where $C(X)$ is a positive number depending only on X. Moreover denoting $X^{\Lambda}(t) = \gamma_t^{\Lambda}(X)$ one has for $t \in [-T, T]$

$$\begin{aligned} |q_i^{\Lambda}(t) - q_i| &\leqslant \int_0^t ds \left[G(X^{\Lambda}(t))\, \varphi(q_i^{\Lambda}(s)) \right]^{1/2} \\ &\leqslant e^T \sqrt{\varphi_i}\,(T) C(X) \end{aligned} \tag{5.8}$$

where $\varphi_i(T) = \sup[\varphi(q_i(s)) \mid |s| < T]$. On the other hand one also obtains

$$\varphi_i(T) \leqslant C_2 \varphi(q_i) \tag{5.9}$$

$C_2 > 0$ depending only on X and T. The uniform control (in Λ) of the displacements allows us to apply the techniques of Refs. 7 and 10 (Ref. 15 for long-range potential) in order to prove the following theorem:

Theorem 5.1. For all X for which $\tilde{G}_\infty(X) < +\infty$, there exists a solution $X \to X(t)$ of the Newton equations satisfying

$$\frac{|q_i(t) - q_i|}{\varphi(q_i)} \leqslant H < +\infty \tag{5.10}$$

for some $H > 0$. Moreover such a solution is unique in the class of all solutions satisfying (5.10) and it yields

$$X(t) = \lim_{\Lambda \to \infty} \gamma_t^\Lambda(X) \tag{5.11}$$

We underline that the convergence (5.11) (for subsequence) may be proven to hold also for a reasonable sequence of regions,[17,10,14] improving the results of the previous section.

As a final remark, it has to be noticed that a stronger uniqueness theorem than that already stated in Theorem 5.1, is expected to hold. More precisely one would be able to prove that there is only one flow of measures $\{\gamma_t \mu\}_{t \in \mathbb{R}}$ satisfying Eq. (4.14) and regularity conditions as superstability estimates, for each time. Such a problem seems quite connected with the one treated in Ref. 12, but it does not seem easy to combine the techniques of such a paper with the results presented here.

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