Thermodynamic Limit of Time-Dependent Correlation Functions for One-Dimensional Systems

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We investigate the time evolution of the correlation functions of a nonequilibrium system when the size of the system becomes very large. At the initial time $t = 0$, the system is represented by an equilibrium grand canonical ensemble with a Hamiltonian consisting of a kinetic energy part, a pairwise interaction potential energy between the particles, and an external potential. At time $t = 0$ the external field is turned off and the system is permitted to evolve under its internal Hamiltonian alone. Using the "time-evolution theorem" for a 1-dimensional system with bounded finite-range pair forces, we prove the existence of infinite-volume time-dependent correlation functions for such systems, $\lim \rho_\Lambda(t; q_1, p_1; \cdots; q_n, p_n)$, as $\Lambda \to \infty$, where Λ is the size of the finite system. We also show that these infinite-volume correlation functions satisfy the infinite BBGKY hierarchy in the sense of distributions.

1. INTRODUCTION

The rigorous mathematical study of equilibrium statistical mechanics during the last decade has achieved many successes. This study concerns itself primarily with the properties of equilibrium systems in the thermodynamic limit, i.e., as the size of the system becomes infinite at fixed temperature and activity (or density). In particular, the existence and analyticity of the correlation functions at small values of the activity z has been proven for a wide class of interacting systems.[1] The existence and convexity of the free energy has been proven for an even larger class of systems at all values of the activity.[2]

The comparable mathematical investigation of the infinite-volume limit of nonequilibrium systems is much more difficult and has begun only recently. The results are restricted to 1-dimensional systems of particles interacting by smooth, finite-range pair forces, and they prove the existence for all times of a "regular" solution of Newton's equations of motion for a "regular" initial configuration. A regular configuration is, roughly speaking, one in which the number of particles in a unit interval and the magnitude of the momentum of any particle in that interval have a bound of the form $\delta \log R$, where R denotes the distance of the interval from the origin. It is shown in Ref. 3 that, at equilibrium, if either the activity is small or the interparticle potential is positive, the set of nonregular configuration has probability zero.

A question left open by these results is whether a state which at time $t = 0$ is described by a set of correlation functions can still be described by a set of correlation functions when $t \neq 0$.

In this paper we investigate this question and prove that, for certain classes of initial states, the time-evolving state is described by correlation functions and that these correlation functions satisfy the BBGKY hierarchy in the sense of distributions [see (2.9)].

The initial states we consider can be described as follows: Suppose that the system is in equilibrium at temperature β^{-1} and activity z under the influence of a pair potential and an external potential h which is localized in a finite region I_h. At time $t = 0$, we switch off the external field and the system begins to evolve. We prove that, if the activity is sufficiently small (i.e., if we are deep inside the gaseous phase), the system can always be described by a set of correlation functions which vary in time according to the BBGKY hierarchy. We are unable to prove even that the time-averaged correlation functions evolve toward the correlation functions which correspond to the equilibrium state at temperature β^{-1} and activity z (in absence of external field), as would be expected. We are, however, able to prove that the time-averaged correlation functions converge to a limit satisfying the stationary BBGKY hierarchy.

We note that initial states of the kind just described suffice, in principle, for the study of transport properties at low activity.

2. DESCRIPTION OF INITIAL STATE AND SUMMARY OF RESULTS

We consider a 1-dimensional system of identical particles of unit mass, interacting through a stable pair-potential $\Phi(q)$ which has finite range and is

twice continuously differentiable. We denote

$$C = -\inf_{n, q_1, \cdots, q_n} \left(n^{-1} \sum_{i<j} \Phi(q_i - q_j) \right). \qquad (2.1)$$

The condition of stability says precisely that $C < \infty$; it guarantees that the thermodynamic functions are well defined.[1]

The initial states we consider will be equilibrium states, at inverse temperature β and chemical potential μ, for an interaction coming from the pair potential Φ and an external potential $h(q)$ which is continuous and which vanish outside some bounded interval I_h. We will assume that the activity z [$= e^{\mu\beta}(2\pi/\beta)^{\frac{1}{2}}$, in units where Planck's constant is unity] is small enough so that the Mayer series converges, i.e.,

$$z < B(\beta)^{-1} \exp\left(-\beta C - 1\right), \qquad (2.2)$$

where

$$B(\beta) = \int dq \, |\exp\left[-\beta\Phi(q)\right] - 1|. \qquad (2.3)$$

Under these conditions, the thermodynamic limit for the correlation functions is known to exist for $h = 0$.[1,4]

Now let Λ denote a finite interval centered at the origin and containing I_h, and let

$$H_\Lambda(q_1, p_1; \cdots; q_n, p_n) = \tfrac{1}{2} \sum_{i=1}^{n} p_i^2 + \sum_{i<j} \Phi_\Lambda(q_i - q_j) \qquad (2.4)$$

denote the Hamiltonian for a system of n particles, in the box Λ with periodic boundary conditions, interacting by the periodized 2-body interaction Φ_Λ. (By Φ_Λ we mean the potential obtained by periodizing Φ with respect to Λ. In order that Φ_Λ be unambiguous, we will assume that the length of Λ is at least twice the range of Φ.[3]) We let $\tilde{T}_\Lambda^t$ denote the time-evolution mapping in the periodic box Λ determined by the Hamiltonian H_Λ. Finally, we let

$$h(q_1, \cdots, q_n) = \sum_{i=1}^{n} h(q_i). \qquad (2.5)$$

Here it is convenient to introduce a piece of notation. Instead of writing $(q_1, p_1; \cdots; q_n, p_n)$ for a point of $(R^2)^n$, we will write $(x)_n$. If

$$(x)_n = (q_1, p_1; \cdots; q_n, p_n)$$

and if

$$(y)_m = (q_1', p_1'; \cdots; q_m', p_m'),$$

we use $(x)_n \cup (y)_m$ to denote

$$(q_1, p_1; \cdots; q_n, p_n; q_1', p_1'; \cdots; q_m', p_m') \in (R^2)^{n+m}.$$

We also write $d(x)_n$ for $dq_1 dp_1 \cdots dq_n dp_n$.

We now want to consider the following situation: We start at time $t = 0$ with the equilibrium state in the

box Λ with inverse temperature β and chemical potential μ (and the external potential h as well as the interparticle potential Φ). We let the state evolve in time with $\tilde{T}_\Lambda^t$ (without the external potential); we write down the correlation functions for the time-evolved state; and we study their behavior as $\Lambda \to \infty$. Physically, this situation corresponds to having a system in equilibrium in the presence of an external potential h, turning off the external potential at $t = 0$, and watching the evolution of the correlations functions as $\Lambda \to \infty$.

Thus, we want to examine the correlation functions[5]:

$$\rho_\Lambda(t; (x)_n) = \frac{1}{\Xi_\Lambda} \sum_{m=0}^{\infty} \frac{e^{\beta\mu(m+n)}}{m!} \int_{(\Lambda \times R)^m} d(x')_m \times \exp\left\{-\beta(H_\Lambda + h)[\tilde{T}_\Lambda^{-t}((x)_n \cup (x')_m)]\right\}, \qquad (2.6)$$

where

$$\Xi_\Lambda = \sum_{m=0}^{\infty} \frac{e^{\beta\mu m}}{m!} \int_{(\Lambda \times R)^m} d(x')_m \exp\left\{-\beta(H_\Lambda + h)[(x')_m]\right\}. \qquad (2.7)$$

Our main results can be stated as follows:

(i) If h is nonnegative, the limit as $\Lambda \to \infty$ of $\rho_\Lambda(t; (x)_n)$ exists for all t and $(x)_n$.

(ii) If h is not assumed to be nonnegative, the limit as $\Lambda \to \infty$ of $\rho_\Lambda(t; (x)_n)$ exists in the sense of distributions in $(x)_n$ for each t; the limiting distribution is actually a locally square-integrable function of $(x)_n$. In either case, we will denote the limit by $\rho(t; (x)_n)$.

(iii) The infinite-volume correlation functions $\rho(t; (x)_n)$ satisfy the BBGKY hierarchy in the following form: For any C^1 function $f(x)_n$ of compact support on $(R^2)^n$, we let

$$\rho_t(f) = \int_{(R^2)^n} \rho(t; (x)_n) f(x)_n \, d(x)_n. \qquad (2.8)$$

Then $\rho_t(f)$ is a differentiable function of t and

$$\frac{d}{dt} \rho_t(f) = \rho_t(\{H, f\}) - \rho_t(f_1), \qquad (2.9)$$

where

$$\{H, f\}(q_1, p_1; \cdots; q_n, p_n) = \sum_{i=1}^{n} \left(\frac{\partial H}{\partial p_i} \frac{\partial f}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial f}{\partial p_i} \right), \qquad (2.10)$$

$$f_1(q_1, p_1; \cdots; q_{n+1}, p_{n+1}) = \sum_{i=1}^{n} \frac{\partial \Phi(q_i - q_{n+1})}{\partial q_i} \frac{\partial f}{\partial p_i}, \qquad (2.11)$$

$$H(q_1, p_1; \cdots; q_n, p_n) = \tfrac{1}{2} \sum_{i=1}^{n} p_i^2 + \sum_{i<j} \Phi(q_i - q_j). \qquad (2.12)$$

Equation (2.9) may be obtained from the standard formal BBGKY hierarchy[5] by multiplying by the test function $f(x)_n$, integrating over (x_n), and putting the q and p derivatives on the test function by integration by parts.

(iv) If $\rho_0(x)_n$ denotes the equilibrium correlations with no external potential, then for all $n, m > 0$

$$\lim_{a \to \infty} \rho(t; q_1, p_1; \cdots; q_n, p_n;$$

$$q_{n+1} + a, p_{n+1}; \cdots; q_{n+m} + a, p_{n+m})$$

$$= \rho(t; q_1, p_1; \cdots; q_n, p_n)$$

$$\times \rho_0(q_{n+1}, p_{n+1}; \cdots; q_{n+m}, p_{n+m}). \quad (2.13)$$

3. INFINITE SYSTEMS

Although we did not need the theory of actually infinite systems to formulate our results, the proofs depend on this theory. We will summarize in this section the main results that we need. For more details, see Refs. 1 or 3.

A locally finite configuration of particles is defined by giving a sequence (possibly finite) of positions and momenta (q_i, p_i) such that each bounded interval in R contains only finitely many q_i. However, since the particles are supposed to be identical, we identify configurations which differ only by the labeling of the particles. Thus, a configuration may be thought of as subset of phase space R^2 with multiplicity, where the subset is just the set of occupied points and the multiplicity of each point is the number of particles at the point. We will let $\mathfrak{X}$ denote the set of all such configurations. If X and Y are configurations belonging to $\mathfrak{X}$, we let $X \cup Y$ be the configuration obtained by adding the multiplicities for X and Y. Also, if $\Lambda \subset R$, and if $X \in \mathfrak{X}$, we let $X \cap \Lambda$ denote the configuration obtained from $\mathfrak{X}$ by omitting all particles whose positions are not in Λ. The set of configurations with all particles in Λ will be denoted by $\mathfrak{X}(\Lambda)$.

We will say that a function f on $\mathfrak{X}$ is *measurable in* Λ if

$$f(X) = f(X \cap \Lambda)$$

for all $X \in \mathfrak{X}$. There is a simple way to construct such functions. Let ψ be a function on R^2 such that $\psi(q, p) = 0$ for $q \notin \Lambda$. Then define

$$(\textstyle\sum \psi)(X) = \sum_i \psi(q_i, p_i),$$

where X is determined by (q_i, p_i). If Λ is bounded, there are only finitely many nonzero terms in this sum. Clearly, $\sum \psi$ is measurable in Λ. We give $\mathfrak{X}$ the weakest topology such that $\sum \psi$ is continuous for all continuous $\psi(q, p)$ whose support in q is bounded. It can be convincingly argued that states of classical statistical mechanics should be identified with Borel probability measures on $\mathfrak{X}$ (see Ref. 6).

If Λ is a bounded open subset of R, the mapping $X \to X \cap \Lambda$ is Borel from $\mathfrak{X}$ to $\mathfrak{X}(\Lambda)$. A Borel measure γ on $\mathfrak{X}$ defines therefore a measure γ_Λ on $\mathfrak{X}(\Lambda)$, i.e., a sequence $\gamma_{n,\Lambda}$ of symmetric Borel measures on $(\Lambda \times R)^n$, $n = 0, 1, 2, \cdots$. If each $\gamma_{n,\Lambda}$ is absolutely continuous with respect to Lebesgue measure, we define *density distributions* $f_\Lambda(x)_n$ by

$$d\gamma_{n,\Lambda} = f_\Lambda(x)_n \, d(x)_n / n!, \quad (3.1)$$

where $f_\Lambda(x)_n / n!$ is the probability density of finding precisely n particles with position $q_1, \cdots, q_n$ in Λ and momenta $p_1, \cdots, p_n$.

For any symmetric continuous function ψ on $(R^2)^n$, with compact support, we define a function $\sum \psi$ on $\mathfrak{X}$ by

$$\sum \psi(X) = \sum_{i_1 < i_2 < \cdots < i_n} \psi(q_{i_1}, p_{i_1}; \cdots; q_{i_n}, p_{i_n}), \quad (3.2)$$

where the configuration X is defined by (q_i, p_i). If γ is a measure on $\mathfrak{X}$ such that $\sum \psi$ is γ-integrable for all such $\psi(x)_n$, then

$$\psi \to \int d\gamma (\textstyle\sum \psi)$$

is a positive linear functional on the space of continuous symmetric functions on $(R^2)^n$ of compact support, i.e., a symmetric measure on $(R^2)^n$. When this measure exists and is absolutely continuous with respect to Lebesgue measure, so that it can be written $\rho(x)_n \, d(x)_n / n!$, we say that $\rho(x)_n$ is the nth correlation function of γ. To recapitulate: The correlation function $\rho(x)_n$ is defined by the relation

$$\int \psi(x)_n \rho(x)_n \frac{d(x)_n}{n!} = \int \textstyle\sum \psi(X) \, d\gamma(X). \quad (3.3)$$

It is not hard to see that, if γ has correlation functions of all orders, then density distributions exist and, for $q_1, \cdots, q_n \in \Lambda$,

$$\rho(q_1, p_1; \cdots; q_n, p_n)$$

$$= \sum_{m=0}^{\infty} \int_{(\Lambda \times R)^m} \frac{dq_1' \, dp_1' \cdots dq_m' \, dp_m'}{m!}$$

$$\times f_{\Lambda, n+m}(q_1, p_1; \cdots; q_m', p_m'). \quad (3.4)$$

Conversely, if there exists a constant η such that, for all Λ and n,

$$\int_{(\Lambda \times R)^n} d(x)_n \rho(x)_n \le [\eta V(\Lambda)]^n, \quad (3.5)$$

$V(\Lambda)$ being the length of the interval Λ, the density distributions can be reexpressed in terms of the

correlation functions by

$$f_\Lambda(x)_n = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!} \int_{(\Lambda \times R)^m} d(y)_m \rho((x)_n \cup (y)_m). \quad (3.6)$$

It has been shown[1] that, for activities satisfying (2.2), the infinite-volume limits of the correlation functions for finite-volume equilibrium ensembles exist; they have the form

$$\rho(q_1, p_1; \cdots; q_n, p_n)$$
$$= \rho(q_1, \cdots, q_n) \exp\left[-\tfrac{1}{2}\beta(p_1^2 + \cdots + p_n^2)\right], \quad (3.7)$$

where, for some real number ξ,

$$\rho(q_1, \cdots, q_n) \le \xi^n \quad (3.8)$$

for all n, $q_1, \cdots, q_n$, and hence they satisfy an estimate of the form (3.5). Thus, a measure on $\mathfrak{X}$ may be reconstructed from this set of correlation functions; we denote this measure γ_0 and call it the infinite-volume equilibrium state. It follows easily from the estimates in Ref. 7 that, if ψ is a bounded Borel function on $\mathfrak{X}$ measurable in some bounded set, then

$$\int d\gamma_0 \psi = \lim_{\Lambda \to \infty} \int_{\mathfrak{X}(\Lambda)} d\gamma_{(\Lambda)} \psi, \quad (3.9)$$

where $\gamma_{(\Lambda)}$ is the finite-volume grand canonical ensemble density [regarded as a probability measure on $\mathfrak{X}(\Lambda)$].

4. THE EVOLUTION THEOREM

In this section we summarize the results of Ref. 3 in a form convenient for our purposes.

(i) The existence of a solution of the equations of motion has not been established for arbitrary initial data in $\mathfrak{X}$, but only for a special set $\hat{\mathfrak{X}}$ of configurations. This set $\hat{\mathfrak{X}}$ may be written as the union of a family of subsets $\hat{\mathfrak{X}}_\delta$, where δ runs through the positive real numbers. We have

$$\hat{\mathfrak{X}}_\delta \supset \hat{\mathfrak{X}}_{\delta'}, \quad \delta \ge \delta'.$$

Each $\hat{\mathfrak{X}}_\delta$ is compact in $\mathfrak{X}$. The sets $\hat{\mathfrak{X}}_\delta$ are large in the sense that

$$\gamma_0(\hat{\mathfrak{X}}) = 1, \quad \text{i.e.,} \quad \lim_{\delta \to \infty} \gamma_0(\mathfrak{X} \setminus \hat{\mathfrak{X}}_\delta) = 0.$$

In fact, a slightly stronger statement is true

$$\lim_{\delta \to \infty} \gamma_{(\Lambda)}(\mathfrak{X}(\Lambda) \cap \hat{\mathfrak{X}}_\delta) = 1$$

uniformly in Λ for large Λ.

(ii) The crux of the existence of time evolution is contained in the following statement: There is a 1-parameter group of mappings T^t of $\hat{\mathfrak{X}}$ onto itself such that, for any continuous function ψ on $\mathfrak{X}$ which is measurable in some bounded interval,

$$\lim_{\Lambda \to \infty} \psi(\tilde{T}_\Lambda^t(X \cap \Lambda)) = \psi(T^t X)$$

for $X \in \hat{\mathfrak{X}}$. The convergence is uniform for X in any fixed $\hat{\mathfrak{X}}_\delta$ and t in any bounded interval.[8] For any fixed δ, $(t, X) \to T^t X$ is continuous from $R \times \hat{\mathfrak{X}}_\delta$ to $\mathfrak{X}$. If an appropriate labeling of the particles in

$$T^t X = (q_1(t), p_1(t), q_2(t), \cdots)$$

is chosen, then the $(q_i(t), p_i(t))$ solve the differential equations

$$\frac{dq_i(t)}{dt} = p_i(t), \quad \frac{dp_i(t)}{dt} = \sum_{j \ne i} \Phi'(q_i(t) - q_j(t)).$$

(iii) The mapping $(X, X') \to X \cup X'$, sending $\mathfrak{X} \times \mathfrak{X}$ to $\mathfrak{X}$, is continuous. If $X \in \hat{\mathfrak{X}}_\delta$ and $X' \in \hat{\mathfrak{X}}_{\delta'}$, then $X \cup X' \in \hat{\mathfrak{X}}_{\delta+\delta'}$.

(iv) Every point in $(R^2)^n$ determines a point in $\mathfrak{X}$ representing a configuration of exactly n particles. We will usually fail to distinguish between $(x)_n$ as a point of $(R^2)^n$ and the corresponding point in $\mathfrak{X}$. The mapping from $(R^2)^n$ to $\mathfrak{X}$ so defined is continuous and the image of each bounded set is contained in some $\hat{\mathfrak{X}}_\delta$.

(v) The equilibrium measure γ_0 on $\hat{\mathfrak{X}}$ (more precisely, the measure obtained by restricting γ_0 to $\hat{\mathfrak{X}}$) is invariant under T^t for all t; i.e., if $E \subset \hat{X}$ is a Borel set, then

$$\gamma_0(E) = \gamma_0(T^{-t}E).$$

5. INFINITE-VOLUME LIMITS OF TIME-DEPENDENT QUANTITIES

Proposition 1: Let ϕ and ψ be functions on $\mathfrak{X}$, both measurable in some bounded interval I. We assume ϕ to be continuous and ψ to be a Borel function. We also assume that, for some real number α,

$$|\phi(X)| \le \exp[\alpha N_I(X)], \quad (5.1)$$

$$|\psi(X)| \le \exp[\alpha N_I(X)] \quad (5.2)$$

[where $N_I(X)$ is the number of particles in the interval I for the configuration X]. Then
(i) $\psi(Y)\phi(T^t Y)$ is γ_0 integrable and

$$\int_\mathfrak{X} d\gamma_0(Y)\psi(Y)\phi(T^t Y)$$

$$= \lim_{\Lambda \to \infty} \int_{\mathfrak{X}(\Lambda)} d\gamma_{(\Lambda)}(Y)\psi(Y)\phi(\tilde{T}_\Lambda^t Y). \quad (5.3)$$

(ii) If ϕ is further assumed to be bounded, then, for any $(x)_n \in (R^2)^n$, $\psi(Y)\phi(T^t(Y \cup (x)_n))$ is γ_0 integrable, and

$$\int_{\mathfrak{X}} d\gamma_0(Y)\psi(Y)\phi(T^t(Y \cup (x)_n))$$
$$= \lim_{\Lambda \to \infty} \int_{\mathfrak{X}(\Lambda)} d\gamma_{(\Lambda)}(Y)\psi(Y)\phi(\tilde{T}^t_\Lambda(Y \cup (x)_n)). \quad (5.4)$$

The integral varies continuously with $(x)_n$.

Proof: There exists a real number ξ such that the nth correlation function of $\gamma_{(\Lambda)}$, $\rho_\Lambda(x)_n$ satisfies

$$\rho_\Lambda(x)_n \leq \xi^n \exp\left(-\tfrac{1}{2}\beta \sum_{i=1}^{n} p_i^2\right),$$
$$(x)_n = (q_1, p_1; \cdots; q_n, p_n) \quad (5.5)$$

for all n, $(x)_n$, and all sufficiently large Λ. This inequality persists for the infinite-volume correlation functions. By (3.6), the probability of finding precisely N particles in I, with respect to any $\gamma_{(\Lambda)}$ or with respect to γ_0, is majorized by

$$(n!)^{-1}[\xi(2\pi/\beta)^{\frac{1}{2}}V(I)]^n \exp[\xi(2\pi/\beta)^{\frac{1}{2}}V(I)]. \quad (5.6)$$

It follows that $\exp[\alpha N_I(Y)]$ is square-integrable with respect to each $\gamma_{(\Lambda)}$ and with respect to γ_0 and that its square-integral has an upper bound which is independent of Λ. By (5.1) and (5.2), ϕ and ψ are both γ_0 square-integrable and, since γ_0 is invariant under T^t, $\psi \circ T^t$ is also γ_0 square-integrable. By the Schwarz inequality, then, $\psi(Y)\phi(T^t Y)$ is γ_0-integrable. Similarly, if ϕ is bounded, $\psi(Y)\phi(T^t(Y \cup (x)_n))$ is γ_0 integrable. By 4(ii)–(iv), $T^t(Y \cup (x)_n)$ varies continuously with $(x)_n$; hence,

$$\int d\gamma_0(Y)\psi(Y)\phi(T^t(Y \cup (x)_n))$$

is a continuous function of $(x)_n$, by the Lebesgue dominated-convergence theorem.

Because of the boundedness of the square-integrals, replacing ϕ by $-\lambda$ if $\phi \leq \lambda$, ϕ if $-\lambda \leq \phi \leq \lambda$, and λ if $\phi \geq \lambda$ with λ large, makes a change in

$$\int d\gamma_{(\Lambda)}\psi(\phi \circ T^t)$$

which is small uniformly in Λ. Hence, in proving (5.3), we can assume that ϕ is bounded. In this case, (5.3) is a special case of (5.4). In a similar way, we see that, in proving (5.4), ψ may also be assumed to be bounded.

To prove (5.4), assuming ψ bounded, we choose $\epsilon > 0$ and then choose δ large enough so that

$$\gamma_{(\Lambda)}(\mathfrak{X}(\Lambda) \setminus \hat{\mathfrak{X}}_\delta) < \epsilon, \quad \text{for all sufficiently large } \delta\Lambda,$$
$$(5.7)$$

and

$$\gamma_0(\mathfrak{X} \setminus \mathfrak{X}_\delta) < \epsilon;$$

this is possible by (i). Now, by 4(ii)–(iv), the mapping

$$Y \to \Phi(T^t(Y \cup (x)_n))$$

is continuous on $\hat{\mathfrak{X}}_\delta$, and $\hat{\mathfrak{X}}_\delta$ is compact in $\mathfrak{X}$. The collection of all functions on $\hat{\mathfrak{X}}_\delta$, which are restrictions of continuous functions on $\mathfrak{X}$ measurable in bounded intervals (the interval may vary with the function), is an algebra of continuous functions on $\hat{\mathfrak{X}}_\delta$ containing the constants and separating points. Hence, by the Stone–Weierstrass theorem,[9] there is a continuous function Φ_1 on $\mathfrak{X}$, measurable in some bounded interval, such that

$$|\phi_1(Y) - \phi(T^t(Y \cup (x)_n))| < \epsilon \quad (5.8)$$

for all $Y \in \hat{\mathfrak{X}}_\delta$. We can also assume

$$\|\phi_1\|_\infty \leq \|\phi\|_\infty. \quad (5.9)$$

Because

$$\lim_{\Lambda \to \infty} \phi(\tilde{T}^t_\Lambda([Y \cup (x)_n] \cap \Lambda)) = \phi(T^t(Y \cup (x)_n))$$

uniformly for $Y \in \hat{\mathfrak{X}}_\delta$ (by 4(ii)), we have

$$|\phi_1(Y) - \phi(\tilde{T}^t_\Lambda(Y \cup (x)_n))| < \epsilon \quad (5.10)$$

for all sufficiently large Λ and all $Y \in \hat{\mathfrak{X}}_\delta \cap \mathfrak{X}(\Lambda)$.

Now

$$\left| \int_{\mathfrak{X}} d\gamma_0(Y)\psi(Y)\phi(T^t(Y \cup (x)_n)) \right.$$
$$\left. - \int_{\mathfrak{X}(\Lambda)} d\gamma_{(\Lambda)}\psi(Y)\phi(\tilde{T}^t_\Lambda(Y \cup (x)_n)) \right|$$
$$\leq \left| \int_{\mathfrak{X}} d\gamma_0(y)\psi(Y)[\phi(T^t(Y \cup (x)_n)) - \phi_1(Y)] \right|$$
$$+ \left| \int_{\mathfrak{X}} d\gamma_0(Y)\psi(Y)\phi_1(Y) - \int_{\mathfrak{X}(\Lambda)} d\gamma_{(\Lambda)}(Y)\psi(Y)\phi_1(Y) \right|$$
$$+ \left| \int_{\mathfrak{X}(\Lambda)} d\gamma_{(\Lambda)}(Y)\psi(Y)[\phi_1(Y) - \phi(\tilde{T}^t_\Lambda(Y \cup (x)_n))] \right|.$$
$$(5.11)$$

The first term on the right of (5.11) is majorized by

$$\left| \int_{\hat{\mathfrak{X}}_\delta} d\gamma_0(Y)\psi(Y)[\phi(T^t(Y \cup (x)_n)) - \phi_1(Y)] \right|$$
$$+ \left| \int_{\mathfrak{X} \setminus \hat{\mathfrak{X}}_\delta} d\gamma_0(Y)\psi(Y)[\phi(T^t(Y \cup (x)_n)) - \phi_1(Y)] \right|$$
$$\leq \|\psi\|_\infty \epsilon + \epsilon \|\psi\|_\infty(2\|\phi\|_\infty) = \epsilon \|\psi\|_\infty(1 + 2\|\phi\|_\infty).$$

[We have used (5.7), (5.8), and (5.9).] Similar arguments show that the same quantity majorizes the the third term on the right of (5.11) provided that Λ

is large enough so that (5.10) holds. Finally, the middle term on the right of (5.11) approaches zero as $\Lambda \to \infty$ by (3.9). Hence, for Λ sufficiently large,

$$\left| \int_{\mathfrak{X}} d\gamma_0(Y)\psi(Y)\phi(T^t(Y \cup (x)_n)) \right.$$
$$\left. - \int_{\mathfrak{X}(\Lambda)} d\gamma_{(\Lambda)}(Y)\psi(Y)\phi(\tilde{T}_\Lambda^t(Y \cup (x)_n)) \right|$$
$$\leq 3\epsilon \|\psi\|_\infty (1 + 2\|\phi\|_\infty).$$

Since $\epsilon > 0$ is arbitrary, (5.4) follows.

Corollary 1: Assume the external potential h is nonnegative, and let the time-dependent finite-volume correlation functions be defined as in (2.6). Then

$$\lim_{\Lambda \to \infty} \rho_\Lambda(t; (x)_n)$$

exists for all t and $(x)_n$ and the convergence is locally uniform in $(x)_n$. Furthermore,

$$\lim_{\Lambda \to \infty} \rho_\Lambda(t; (x)_n) = e^{\beta \mu n} \int_{\mathfrak{X}} d\gamma_0(Y)$$
$$\times \exp\left[-\beta \sum h(T^{-t}(Y \cup (x)_n))\right]$$
$$\times \exp\{-\beta[H(x)_n + W((x)_n, Y)]\}$$
$$\times \left(\int_{\mathfrak{X}} d\gamma_0(Y)e^{-\beta \Sigma h(Y)}\right)^{-1}, \quad (5.12)$$

where

$$W((x)_n, Y) = \sum_{i,j} \phi(q_i - q_j');$$

$Y = (q_i', p_i')$, and the limit is a continuous function of $(x)_n$.

Proof: From the definition of $\rho_\Lambda(t; (x)_n)$ and the fact that

$$H_\Lambda \circ \tilde{T}_\Lambda^t = H_\Lambda$$

(conservation of energy), it follows that

$$\rho_\Lambda(t; (x)_n) = e^{\beta \mu n} \int_{\mathfrak{X}(\Lambda)} d\gamma_{(\Lambda)}(Y)$$
$$\times \exp\left[-\beta \sum h(\tilde{T}_\Lambda^t(Y \cup (x)_n))\right]$$
$$\times \exp\{-\beta[H(x)_n + W((x)_n, Y)]\}$$
$$\times \left(\int_{\mathfrak{X}(\Lambda)} d\gamma_{(\Lambda)}(Y)e^{-\beta \Sigma h(Y)}\right)^{-1}; \quad (5.13)$$

the corollary then follows by straightforward application of Proposition 1.

Corollary 2: Let the time-dependent finite-volume correlation functions be defined as in (2.6), and let the external potential h be any continuous function of

compact support. Let $f(x)_n$ be any continuous function of compact support on $(R^2)^n$. Then

$$\lim_{\Lambda \to \infty} \int \frac{d(x)_n}{n!} \rho_\Lambda(t; (x)_n)f(x)_n$$
$$= \int d\gamma_0(Y) \exp\left[-\beta(\sum h)(T^{-t}Y)\right](\sum f)(Y)$$
$$\times \left(\int d\gamma_0(Y)e^{-\beta \Sigma h(Y)}\right)^{-1}; \quad (5.14)$$

moreover, there exist locally square-integrable functions $\rho(t; (x)_n)$ such that

$$\lim_{\Lambda \to \infty} \int \frac{d(x)_n}{n!} \rho_\Lambda(t; (x)_n)f(x)_n$$
$$= \int \frac{d(x)_n}{n!} \rho(t; (x)_n)f(x)_n, \quad (5.15)$$

for all continuous f of compact support.

Proof: Again, by the definition of the finite-volume correlation functions and the conservation of energy, we have

$$\int \frac{d(x)_n}{n!} \rho_\Lambda(t; (x)_n)f(x)_n$$
$$= \int d\gamma_{(\Lambda)}(Y) \exp\left[-\beta \sum h(\tilde{T}_\Lambda^{-t}Y)\right] \sum f(Y)$$
$$\times \left(\int d\gamma_{(\Lambda)}(Y)e^{-\beta \Sigma h(Y)}\right)^{-1}; \quad (5.16)$$

thus (5.14) follows from Proposition 1. The existence of the infinite-volume correlation functions $\rho(t; (x)_n)$ as locally square-integrable functions (and not merely as measures) follows from the fact, easily verified, that, if Ω is any bounded open set in $(R^2)^n$, the mapping $f \to \sum f$ from the space of continuous functions with support in Ω to the space of continuous functions on $\mathfrak{X}$ extends to a continuous mapping from $L^2(\Omega, d(x)_n)$ to $L^2(\mathfrak{X}, d\gamma_0)$. Hence, since $e^{-\Sigma h(\cdot)} \in L^2(\mathfrak{X}, d\gamma_0)$, the mapping

$$f \to \lim_{\Lambda \to \infty} \int \frac{d(x)_n}{n!} f(x)_n \rho_\Lambda(t; (x)_n)$$

extends to a continuous linear functional on $L^2(\Omega)$ and is therefore given by a function square-integrable on Ω.

6. THE BBGKY HIERARCHY

Theorem 1: Let ψ be a nonnegative function on $\mathfrak{X}$ with

$$\int \psi(Y) \, d\gamma_0(Y) = 1 \quad \text{and} \quad \int \psi(Y)^2 \, d\gamma_0(Y) < \infty.$$

Let γ denote the probability measure $\psi(Y)\,d\gamma_0(Y)$ on $\mathfrak{X}$, and let γ^t be the time-evolved measure defined by

$$\int \phi(Y)\,d\gamma^t(Y) = \int \phi \circ T^t(Y)\,d\gamma(Y). \quad (6.1)$$

Then γ^t has correlation functions of all orders, and these correlation functions are locally square-integrable. Moreover, for any function f which is infinitely differentiable and of compact support on $(R^2)^n$, $\int d\gamma^t \sum f$ is a differentiable function of t, and

$$\frac{d}{dt}\int \sum f\,d\gamma^t = \int \sum (\{H,f\})\,d\gamma^t - \int \sum f_1\,d\gamma^t, \quad (6.2)$$

where the notation is defined in (2.10)–(2.12).

Proof: By a simple calculation, using the invariance of γ_0 under T^t, we have

$$d\gamma^t = (\psi \circ T^t)\,d\gamma_0,$$
$$\int d\gamma_0\,|\psi \circ T^t|^2 = \int d\gamma_0\,|\psi|^2 < \infty.$$

Thus γ^t is obtained from γ_0 by multiplication by a square-integrable function. The arguments used in the proof of Corollary 2 show that this implies that γ^t has locally square-integrable correlation functions of all orders. On the other hand,

$$\int \sum f\,d\gamma^t = \int \sum [f \circ T^t(Y)]\psi(Y)\,d\gamma_0(Y). \quad (6.3)$$

It follows readily from 4.(ii) that, for any infinitely differentiable f and $Y \in \hat{\mathfrak{X}}$,

$$\frac{d}{dt}\sum f(T^t Y) = \sum (\{H,f\})(T^t Y) - \sum f_1(T^t Y). \quad (6.4)$$

The right-hand side of this expression may be verified to be γ_0-square-integrable; hence, its absolute value is γ integrable, and the integral is a bounded function of t. The complement of $\hat{\mathfrak{X}}$ has γ-measure zero. Hence, by standard theorems about differentiation under the integral sign,

$$\frac{d}{dt}\int \sum f\,d\gamma^t = \int [\sum (\{H,f\}) - \sum f_1]\,d\gamma^t, \quad (6.5)$$

which is just Eq. (6.2).

Corollary 3: Equation (2.9) holds.

Proof: The $\rho(t;(x)_n)$ are the correlation functions of the measure obtained by evolving in time the measure

$$e^{-\beta\Sigma h(Y)}\,d\gamma_0(Y) \Big/ \int d\gamma_0(Y')e^{-\beta\Sigma h(Y')}$$

[by Sec. 4(iii)], and $e^{-\beta\Sigma h(Y)}$ is γ_0-square-integrable.

7. CLUSTER PROPERTIES

Let τ_a denote the operation of translation by a, acting on $\mathfrak{X}$, i.e., $\tau_a(q_i,p_i) = (q_i + a, p_i)$. The equilibrium state γ_0 is invariant under τ_a and has strong cluster properties under the action of τ_a. For a detailed discussion of these cluster properties, see Ref. 1; we will need the following fact, easily deduced from the results in this reference: If ψ and ϕ are functions on $\mathfrak{X}$ which are γ_0-square-integrable, then

$$\lim_{|a|\to\infty}\int d\gamma_0(Y)\psi(Y)\phi(\tau_a Y)$$
$$= \int d\gamma_0(Y)\psi(Y)\int d\gamma_0(Y)\psi(Y). \quad (7.1)$$

Using this result, we will prove the following:

Theorem 2: Let the $\rho(t;(x)_n)$ be defined as in Corollary 2, and let $\rho_0(x)_n$ denote the nth correlation function of the equilibrium measure γ_0. Then, for continuous symmetric functions $f(x)_n$, $g(y)_m$ of compact support,

$$\lim_{|a|\to\infty}\int d(x)_n\,d(y)_m f(x)_n g(y)_m \rho\,(t;(x)_n \cup \tau_a(y)_m)$$
$$= \int d(x)_n f(x)_n \rho(t;(x)_n)\int d(y)_m g(y)_m \rho_0(y)_m. \quad (7.2)$$

Proof: Let $g_a(y)_m = g(\tau_a(y)_m)$, and let $\mathfrak{X}_a$ be the function on $\mathfrak{X}$ defined by

$$\mathfrak{X}_a((q_i,p_i)) = \frac{1}{(n+m)!}\sum'_{i_1,\cdots,i_{n+m}} f(q_{i_1},p_{i_1};\cdots;q_{i_n},p_{i_n})$$
$$\times g_a(q_{i_{n+1}},\cdots,p_{i_{n+m}}), \quad (7.3)$$

where the sum $\sum'$ is to be taken over all $(n+m)$-tuples of distinct indices. Since f and g both have compact supports, for sufficiently large a,

$$f(q_{i_1},\cdots,p_{i_n})g_a(q_{i_{n+1}},\cdots,p_{i_{n+m}}) = 0$$

if any i_k, $1 \le k \le n$, is equal to any i_e, $n+1 \le e \le n+m$. Hence, for such a,

$$\chi_a((q_i,p_i)) = \frac{1}{(n+m)!}\sum'_{i_1,\cdots,i_n} f(q_i,\cdots,p_{i_n})$$
$$\times \sum'_{i_{n+1}\cdots,i_{n+m}} g_a(q_{i_{n+1}},\cdots,p_{i_{n+m}}),$$
$$\mathfrak{X}_a(Y) = \frac{n!\,m!}{(n+m)!}(\sum f)(Y)(\sum g)(\tau_a Y). \quad (7.4)$$

If we let

$$\psi(Y) = e^{-\beta\Sigma h(Y)}\left(\int d\gamma_0(Y')e^{-\beta\Sigma h(Y')}\right)^{-1}, \quad (7.5)$$

then Corollary 2 and the definition of correlation functions gives

$$\frac{1}{(n+m)!}\int d(x)_n\,d(y)_m f(x)_n g(y)_m \rho\,(t;(x)_n \cup \tau_a(y)_m)$$
$$= \int d\gamma_0(Y)\psi(T^{-t}Y)\mathfrak{X}_a(Y)$$
$$= \frac{n!\,m!}{(n+m)!}\int d\gamma_0(Y)\psi(T^{-t}Y)(\sum f)(Y)(\sum g)(\tau_a Y)$$

$$(7.6)$$

for large a. Since any power of ψ, $\sum f$, or $\sum g$ is γ_0-integrable, it follows from (7.1) that

$$\lim_{|a| \to \infty} \int d(x)_n \, d(y)_m f(x)_n g(y)_m \rho\left(t; (x)_n \cup \tau_a(y)_m\right)$$

$$= n! \, m! \left(\int d\gamma_0(Y) \psi(T^{-t}Y) \sum f(Y) \right)$$

$$\times \left(\int d\gamma_0(Y) \sum g(Y) \right)$$

$$= \left(\int d(x)_n f(x)_n \rho(t; (x)_n) \right)$$

$$\times \left(\int d(y)_m g(y)_m \rho_0(y)_m \right),$$

which is just (7.2).

8. REMARKS

We have seen that the infinite-volume correlation functions $\rho(t; (x)_n)$ are the correlation functions for a measure obtained by multiplying the equilibrium measure γ_0 by $\psi \circ T^{-t}$, where ψ is defined in (7.5). We may define time-averaged correlation functions

$$\bar{\rho}(T, (x)_n) = T^{-1} \int_0^T dt \rho(t; (x)_n); \qquad (8.1)$$

these are the correlation functions of the measure obtained by multiplying γ_0 by

$$\bar{\psi}_T = T^{-1} \int_0^T dt \psi \circ T^{-t}. \qquad (8.2)$$

By the mean ergodic theorem,[10] $\bar{\psi}_T$ converges in $L^2(\chi, d\gamma_0)$ to some limiting function $\bar{\psi}_\infty$ which has γ_0-integral unity and is invariant under T^t. As in the proof of Corollary 2, the measure $\bar{\gamma}_\infty$ obtained by multiplying γ_0 by $\bar{\psi}_\infty$ has locally square-integrable correlation functions $\bar{\rho}(x)_n$. Trivially, we have

$$\int \frac{d(x)_n}{n!} f(x)_n \bar{\rho}_\infty(x)_n =$$

$$\int d\gamma_0 \bar{\psi}_\infty \sum f = \lim_{T \to \infty} \int d\gamma_0 \bar{\psi}_T \sum f$$

$$= \lim_{T \to \infty} \int \frac{d(x)_n}{n!} f(x)_n \bar{\rho}(T; (x)_n), \quad (8.3)$$

i.e.,

$$\bar{\rho}_\infty(x)_n = \lim_{T \to \infty} \bar{\rho}(T; (x)_n) \qquad (8.4)$$

in the sense of distributions.

Moreover, the measure $\bar{\gamma}_\infty$ is time invariant and is obtained by multiplying γ_0 by a square-integrable function. Hence (Theorem 1) its correlation functions must satisfy the stationary BBGKY hierarchy. We have thus shown that the time-averaged correlation functions tend, as $T \to \infty$, to stationary correlation functions. Unfortunately, we do not know that these stationary correlation functions are the equilibrium ones.[11] This would follow if it could be proved that the equilibrium measure γ_0 is ergodic with respect to T^t. The ergodicity of the low-activity equilibrium measures is the outstanding problem in the theory of the time evolution of 1-dimensional systems, and no serious attack has yet been made on it.

Recently, Ruelle[12] has shown that, for a large class of potentials (the so-called superstable potentials) and for arbitrary temperature and activity, the finite-volume correlation functions satisfy an inequality of the form (5.5), where ξ may be chosen to be independent of Λ. One can construct infinite-volume equilibrium measures by taking limits along subsequences of boxes converging to infinity; the equilibrium measures obtained in this way need not be unique (i.e., they may depend on the particular sequence of boxes chosen), but any one of them is concentrated on $\hat{\mathfrak{X}}$, invariant under T^t and has correlation functions satisfying (5.5). It is easy to see that all our results, except those in Sec. 7, extend with appropriate modifications to apply to states obtained by making local perturbations on these equilibrium states.

[1] D. Ruelle, *Statistical Mechanics* (Benjamin, New York, 1969).

[2] J. L. Lebowitz and E. Lieb, Phys. Rev. Letters **22**, 631 (1969).

[3] O. E. Lanford, Commun. Math. Phys. **9**, 126 (1968); **11**, 257 (1969).

[4] The existence of the equilibrium correlation functions for $h \neq 0$ for the systems considered here is a consequence of our general results. It may also be proven independently for all dimensions.

[5] See, for example, N. N. Bogoliubov, J. Phys. USSR **10**, 265 (1946) ("Problems of a Dynamical Theory in Statistical Physics," transl. E. Gora, Providence College, Providence, R.I., 1959.)

[6] D. Ruelle, J. Math. Phys. **8**, 1657 (1967).

[7] D. Ruelle, Ann. Phys. (N.Y.) **25**, 109 (1963).

[8] The last statement, which is the heart of the evolution theorem, means in effect that, if we concentrate our attention on the motion (during a finite time t) of the particles of a given configuration which are initially in a certain finite interval, their motion will not be much affected by the particles initially very far away (the actual size of the "region of influence" will, of course, depend on t and δ). It is this intuitively reasonable statement which provides the key to our ability of controlling the dynamics of our system at least to the extent of proving the rather primitive results of this paper.

[9] L. H. Loomis, *Abstract Harmonic Analysis* (Van Nostrand, Princeton, N.J., 1953).

[10] See P. R. Halmos, *Lectures on Ergodic Theory* (Chelsea, New York, 1956).

[11] The fact that the equilibrium correlation functions, for low activity, satisfy the BBGKY hierarchy even in higher dimensions and for more general potentials has been proven by G. Gallavotti, Nuovo Cimento **52b**, 208 (1968).

[12] D. Ruelle, Commun. Math. Phys., to be published.