

Observables at Infinity and States with Short Range Correlations in Statistical Mechanics

O. E. LANFORD III* and D. RUELLE

I. H. E. S., Bures-Sur-Yvette, France

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Abstract. We say that a representation of an algebra of local observables has short-range correlations if any observable which can be measured outside all bounded sets is a multiple of the identity, and that a state has finite range correlations if the corresponding cyclic representation does. We characterize states with short-range correlations by a cluster property. For classical lattice systems and continuous systems with hard cores, we give a definition of equilibrium state for a specific interaction, based on a local version of the grand canonical prescription; an equilibrium state need not be translation invariant. We show that every equilibrium state has a unique decomposition into equilibrium states with short-range correlations. We use the properties of equilibrium states to prove some negative results about the existence of metastable states. We show that the correlation functions for an equilibrium state satisfy the Kirkwood-Salsburg equations; thus, at low activity, there is only one equilibrium state for a given interaction, temperature, and chemical potential. Finally, we argue heuristically that equilibrium states are invariant under time-evolution.

1. Introduction

The aim of equilibrium statistical mechanics is to describe the equilibrium states of a system, once the interaction between its microscopic components are known. These interactions are usually invariant under a large group G of transformations (the Euclidean group, say, or a translation group) and one may thus assume that an equilibrium state ρ of an infinite system is invariant under G . We say that ρ is G -ergodic if there is no decomposition $\rho = \frac{1}{2} \rho_1 + \frac{1}{2} \rho_2$ where ρ_1 and ρ_2 are distinct states invariant under G . It can be argued that ρ is ergodic if it describes a pure thermodynamic phase and non-ergodic if it describes a mixture¹. The decomposition of G -invariant states into G -ergodic states has received much attention recently².

If one thinks now of an equilibrium state ρ corresponding to a crystal, it appears that the crystal has a symmetry group H_α smaller than the group G under which ρ is invariant. This *spontaneous symmetry*

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¹ For a discussion of this point, see RUELLE [25].

² See for instance DOPLICHER, KASTLER and ROBINSON [5], RUELLE [22], LANFORD and RUELLE [17], STØRMER [27].

breakdown can be understood by writing ρ as a superposition

$$\rho = \int d\alpha \rho_\alpha \quad (1.1)$$

where ρ_α is a state describing a crystal with fixed orientation and lattice position, and $d\alpha$ is a measure on G/H_α . Given an equilibrium state ρ , one may now ask what the prescription is, to find a physically meaningful decomposition like (1.1)³. This problem has been considered by a number of authors⁴ mostly from a group-theoretical viewpoint, and it was suggested by HAAG that the decomposition (1.1) should be into ergodic states for time-evolution⁵.

In the present paper we adopt the point of view that the decomposition (1.1) should distinguish states ρ_α only if they differ "far away" in space; one could say that we look for a decomposition into states ρ_α which differ macroscopically and not just by local fluctuations. We shall say that such states have *short-range correlations* and give them a precise definition in Section 2. In Section 3 we restrict ourselves to classical systems and establish equations which must be satisfied by any equilibrium state. If Δ is the set of states satisfying these equations, it turns out that the states with short-range correlations are just the extremal points of Δ . The results of Sections 3 are used in Section 4 to derive several negative statements about the existence of metastable states in statistical mechanics. In Section 5 we exhibit a case where the invariant equilibrium states already have short range correlations. In Section 6 we give a heuristic argument to show that, for continuous systems, equilibrium states are invariant under time evolution.

Note. After the manuscript of the present article was completed (summer 68), J. LASCoux pointed out to us that results along the same lines had been obtained by R. L. DOBRUSHIN [see *Teorija Verojatn. i ee Prim.* **13**, 201—229 (1968); *Funkts. Analiz i ego Pril.* **2**, 31—43 (1968); **2**, 44—57 (1968); **3**, 27—35 (1969)]. We have not modified our manuscript to take DOBRUSHIN's work into account, but we urge the reader to consult the articles quoted above. It is of particular interest that DOBRUSHIN could prove the existence of a symmetry breakdown for some non-trivial models of a lattice gas [*Funkts. Analiz i ego Pril.* **2**, 44—57 (1968)].

2. Observables at Infinity and States with Short Range Correlations

For the purposes of this section, let \mathfrak{A} be a C^* algebra and let $\{\mathfrak{A}_\Lambda\}$ be a collection of sub C^* -algebras of \mathfrak{A} labelled by the bounded open

³ This decomposition may in some cases (liquid crystals) be into "almost periodic" rather than periodic states ρ_α . Notice that we look for a "natural" decomposition of ρ , not a finest possible decomposition. For a classical system one can decompose ρ into pure states ρ_α where all the positions (and possibly momenta) of all the particles are fixed; this decomposition is too fine to be of interest to us here.

⁴ See in particular KASTLER and ROBINSON [13], ROBINSON and RUELLE [19], DOPLICHER, GALLAVOTTI and RUELLE [4], HAAG, KASTLER, and MICHEL [11].

⁵ R. HAAG, private communication.

subsets of \mathbf{R}^{ν} (continuous systems) or \mathbf{Z}^{ν} (lattice systems). These objects are subject to the restrictions:

QLA 1. $\bigcup_A \mathfrak{A}_A$ is norm-dense in \mathfrak{A} .

QLA 2. If $A \cap M = \emptyset$, and if $A \in \mathfrak{A}_A, B \in \mathfrak{A}_M$ then $[A, B] = 0$.

For any bounded open A , let $\tilde{\mathfrak{A}}_A$ denote the sub C^* -algebra of \mathfrak{A} generated by $\{\mathfrak{A}_M : M \cap A = \emptyset\}$. If \mathfrak{A}_A is interpreted as the algebra of observables measurable inside A , then $\tilde{\mathfrak{A}}_A$ is to be interpreted as the algebra of observables measurable *outside* A . Note that, by QLA 2., \mathfrak{A}_A and $\tilde{\mathfrak{A}}_A$ commute.

Now let π be a $*$ -representation of \mathfrak{A} on a Hilbert space \mathfrak{H}_π , and define

$$\mathfrak{B}_\pi = \bigcap_A \overline{\pi(\tilde{\mathfrak{A}}_A)},$$

where $\overline{\quad}$ denotes weak-operator closure. Since $\overline{\pi(\tilde{\mathfrak{A}}_A)}$ may be interpreted as the algebra of observables (in a generalized sense) measurable outside A , \mathfrak{B}_π may be interpreted as the algebra of observables measurable outside any given bounded open set; we will therefore refer to \mathfrak{B}_π as the *algebra of observables at infinity*. We will say that the representation π has *short range correlations* if the corresponding algebra \mathfrak{B}_π contains only the scalars, and that a state ρ on \mathfrak{A} has *short range correlations* if the corresponding cyclic representation does.

2. 1. Proposition. *For any $*$ -representation π of \mathfrak{A} , the algebra \mathfrak{B}_π is contained in the center of $\overline{\pi(\mathfrak{A})}$.*

Since \mathfrak{B}_π is evidently contained in $\overline{\pi(\mathfrak{A})}$, it suffices by QLA 1. to show that, for any $B \in \mathfrak{B}_\pi$ and any $A \in \mathfrak{A}_A$ for some bounded open A , $[B, A] = 0$. But since $B \in \mathfrak{B}_\pi, B \in \overline{\pi(\tilde{\mathfrak{A}}_A)}$; since $\tilde{\mathfrak{A}}_A$ commutes with \mathfrak{A}_A , the proposition is proved.

It follows at once from this proposition that any factor representation of \mathfrak{A} has short range correlations.

One is most interested in the case in which \mathfrak{A} is one of the C^* -algebras used to describe statistical mechanics. Consider first a one-dimensional classical lattice gas. For such a system, the requirement that a translation-invariant state (i.e., an invariant measure on the space of configurations) have short range correlations is analogous to the requirement that the dynamical system defined by the translation mappings and the invariant measure be a K -system (see SINAI [26] or JACOB [12], Section 10.9). Indeed, ρ defines a K -system if and only if:

$$\bigcap_m \overline{\bigcup_{A \subset (-\infty, -m)} \pi_\rho(\mathfrak{A}_A)} = \{\lambda 1\}$$

or if and only if

$$\bigcap_m \overline{\bigcup_{A \subset (m, \infty)} \pi_\rho(\mathfrak{A}_A)} = \{\lambda 1\};$$

on the other hand, ϱ has finite range correlations if and only if

$$\bigcap_m \overline{\bigcup_{\Lambda \subset (-\infty, -m) \cup (m, \infty)} \pi_\varrho(\mathfrak{A}_\Lambda)} = \{\lambda \mathbf{1}\}.$$

Thus, if ϱ has short range correlations, it defines a K -system, and it seems a plausible conjecture that the converse is also true. In any case, states of classical statistical mechanics having short range correlations may be thought of roughly as multi-dimensional generalizations of K -systems. The following proposition shows, however, that the interpretation is quite different in quantum statistical mechanics: for quantum spin systems, the states with short range correlations are precisely the factor states.

2.2. Proposition. *Let \mathfrak{A} be the quasi-local algebra describing a quantum spin system⁶. Then for any $*$ -representation π of \mathfrak{A} , \mathfrak{B}_π coincides with the center of $\overline{\pi(\mathfrak{A})}$.*

By Proposition 2.1, all we have to show is that any B in the center of $\pi(\mathfrak{A})$ belongs to $\pi(\tilde{\mathfrak{A}}_\Lambda)$ for each bounded Λ . Thus, let B_α be a net of elements of \mathfrak{A} such that $\pi(B_\alpha)$ converges strongly to B . We can suppose that each B_α belongs to some \mathfrak{A}_{M_α} , where $M_\alpha \supset \Lambda$. Now \mathfrak{A}_Λ is a finite matrix algebra; let (e_{ij}) be a set of matrix units for it. Since B commutes with $\pi(\mathfrak{A}_\Lambda)$,

$$B = \sum_i \pi(e_{i1}) B \pi(e_{1i}) = \text{st.}\lim_\alpha \pi \left(\sum_i e_{i1} B_\alpha e_{1i} \right).$$

But $\sum_i e_{i1} B_\alpha e_{1i}$ belongs to \mathfrak{A}_{M_α} and commutes with \mathfrak{A}_Λ ; hence, belongs to $\mathfrak{A}_{M_\alpha} \subset \tilde{\mathfrak{A}}_\Lambda$, so $B \in \overline{\pi(\tilde{\mathfrak{A}}_\Lambda)}$ and the proposition is proved.

A similar argument shows that, if \mathfrak{A} is the quasi-local algebra describing a boson lattice gas or a continuous boson system, \mathfrak{B}_π coincides with the center of $\overline{\pi(\mathfrak{A})}$ provided that the restriction of π to each \mathfrak{A}_Λ is quasi-equivalent to the Fock representation; this will be the case for representations of physical interest (see RUELLE [21], DELL'ANTONIO, DOPLICHER, and RUELLE [3]).

The following proposition shows that, as the terminology suggests, states with short range correlations are characterized by cluster properties. It contains as special cases known results about K -systems (SINAI [26]) and uniformly hyperfinite C^* algebras (POWERS [18], Theorem 2.5);

⁶ By the quasi-local algebra describing a quantum spin system we mean a system $\{\mathfrak{A}, \mathfrak{A}_\Lambda\}$ constructed as follows: Let \mathfrak{H} be a finite-dimensional Hilbert space, \mathfrak{H}_x a copy of \mathfrak{H} for every x in \mathbb{Z}^p , and $\mathfrak{H}_A = \bigotimes_{x \in A} \mathfrak{H}_x$ for every finite $A \subset \mathbb{Z}^p$. Let \mathfrak{A}_A be the algebra of bounded operators on \mathfrak{H}_A . If $A \subset M$, the natural isomorphism $\mathfrak{H}_M = \mathfrak{H}_A \otimes \mathfrak{H}_{M/A}$ identifies \mathfrak{A}_A with a subalgebra of \mathfrak{A}_M . Then \mathfrak{A} is the norm closure of the union of the \mathfrak{A}_Λ 's (i.e., the inductive limit of the \mathfrak{A}_Λ 's). See LANFORD and ROBINSON [15].

the method of proof is a straightforward adaptation of that used in the latter reference.

2.3. Proposition. *Let $\{\mathfrak{A}, \mathfrak{A}_A\}$ be as above, and let ϱ be a state on \mathfrak{A} . Then the following are equivalent:*

1. ϱ has short range correlations.
2. For every $A \in \mathfrak{A}$, there is a bounded open set Λ such that

$$|\varrho(A B) - \varrho(A) \varrho(B)| \leq \|B\|$$

whenever $B \in \mathfrak{A}_\Lambda$.

Assume that 1. holds but that 2. does not. Then there exists $A \in \mathfrak{A}$, an increasing net M_α of bounded open sets whose union is the whole space, and operators $B_\alpha \in \mathfrak{A}_{M_\alpha}$; $\|B_\alpha\| \leq 1$, such that

$$\lim_\alpha \varrho(A B_\alpha) - \varrho(A) \varrho(B) \neq 0 .$$

By passing to a subnet, we can assume that $\pi_\varrho(B_\alpha)$ converges in the weak operator topology; since the limit is in $\bigcap_\alpha \pi(\mathfrak{A}_{M_\alpha})$ it must, by 1., be of the form $b\mathbf{1}$. Then

$$\begin{aligned} \lim_\alpha \varrho(A B_\alpha) - \varrho(A) \varrho(B_\alpha) &= \lim_\alpha [(\Omega_\varrho, \pi_\varrho(A) \pi_\varrho(B_\alpha) \Omega_\varrho) - (\Omega_\varrho, \pi_\alpha(A) \Omega_\varrho) \\ &\quad \times (\Omega_\varrho, \pi_\varrho(B_\alpha) \Omega_\varrho)] \\ &= b(\Omega_\varrho, \pi_\varrho(A) \Omega_\varrho) - b(\Omega_\varrho, \pi_\varrho(A) \Omega_\varrho) = 0 , \end{aligned}$$

contradicting our earlier assumption and proving that 1. implies 2.

Now suppose that 2. holds, and let $B \in \mathfrak{B}_{\pi_\varrho}$. Then

$$|(\Omega_\varrho, \pi_\varrho(A) B \Omega_\varrho) - (\Omega_\varrho, \pi_\varrho(A) \Omega_\varrho) (\Omega_\varrho, B \Omega_\varrho)| \leq \|B\|$$

for all $A \in \mathfrak{A}$. Replacing A by λA multiplies the left-hand side by $|\lambda|$ and leaves the right-hand side unchanged, so the left-hand side must be zero. Letting $b = (\Omega_\varrho, B \Omega_\varrho)$, and using Proposition 2.1, we get therefore:

$$(\pi_\varrho(A_1) \Omega_\varrho, B \pi_\varrho(A_2) \Omega_\varrho) = b(\pi_\varrho(A_1) \Omega_\varrho, \pi_\varrho(A_2) \Omega_\varrho)$$

for all $A_1, A_2 \in \mathfrak{A}$, and hence

$$B = b\mathbf{1} .$$

2.4. Corollary. *Let $\{\mathfrak{A}, \mathfrak{A}_A\}$ be as above and let τ be a representation of the translation group in the automorphism group of \mathfrak{A} such that*

$$\tau_x(\mathfrak{A}_A) = \mathfrak{A}_{A+x} .$$

Let ϱ be a state of \mathfrak{A} which is invariant under τ and which has short range correlations. Let $A_1, \dots, A_n \in \mathfrak{A}$. Then

$$\lim_{\min|x_i - x_j| \rightarrow \infty} \varrho(\tau_{x_1} A_1 \dots \tau_{x_n} A_n) = \varrho(A_1) \dots \varrho(A_n) .$$

We can assume that $A_1, \dots, A_n \in \mathfrak{A}_\Lambda$ for some Λ . Then translation invariance and Proposition 2.3 gives

$$\lim_{\substack{\min_{i \neq j} |x_i - x_j| \rightarrow \infty}} \varrho(\tau_{x_1} A_1 \dots \tau_{x_n} A_n) = \varrho(A_1) \lim_{\substack{\min_{i \neq j} |x'_i - x'_j| \rightarrow \infty}} \varrho(\tau_{x'_2} A_2 \dots \tau_{x'_n} A_n)$$

where $x'_i = x_i - x_1, 2 \leq i \leq n$. The corollary now follows by induction on n .

Because the algebra $\mathfrak{B}_{\pi_\varrho}$ is abelian, it gives a decomposition of the state ϱ . Heuristically, one expects this decomposition to be the coarsest possible decomposition into states with short range correlations. We will not study this decomposition in general. Instead, we will concentrate on the study of the decomposition of equilibrium states of classical statistical mechanics, using special methods to be developed in the next section.

3. Equilibrium Equations for Classical Systems

We shall consider, in this and the following section, only classical lattice gases; in Appendix B we show how our results may be extended to classical hard core continuous systems.

For a lattice gas, $\mathfrak{A} = \mathcal{C}(K)$ is the algebra of continuous complex functions on the compact set⁷

$$K = \{0,1\}^{\mathbf{Z}^v} = \mathcal{P}(\mathbf{Z}^v). \tag{3.1}$$

An element $X : \mathbf{Z}^v \rightarrow \{0,1\}$ of $\{0,1\}^{\mathbf{Z}^v}$ is here identified with the set $\{X \in \mathbf{Z}^v : X(x) = 1\} \in \mathcal{P}(\mathbf{Z}^v)$; K is compact as product of the sets $\{0,1\}$ (which are compact with the discrete topology). If Λ is a finite subset of \mathbf{Z}^v , \mathfrak{A}_Λ is the algebra of "cylindrical functions" A such that for some $\varphi \in \mathcal{C}(\mathcal{P}(\Lambda))$,

$$A(X) = \varphi(X \cap \Lambda) \quad \text{for all } X \in K.$$

If $x \in \mathbf{Z}^v$, τ_x is the automorphism of \mathfrak{A} defined by

$$\tau_x A(X) = A(X - x) \quad \text{for all } X \in \mathcal{P}(\mathbf{Z}^v)$$

where $X - x$ is the set X translated by $-x$.

A state ϱ on \mathfrak{A} is the same thing as a probability measure on K . If Λ is a finite subset of \mathbf{Z}^v , we shall define, for every $X \subset \Lambda$, a measure $\varrho_\Lambda(X, dY)$ on $\mathcal{P}(\mathbf{Z}^v \setminus \Lambda)$ by

$$\varrho(A) = \sum_{X \subset \Lambda} \int A(X \cup Y) \varrho_\Lambda(X, dY). \tag{3.2}$$

We shall say that ϱ is a \mathbf{Z}^v -invariant state, or simply an *invariant state* if

$$\varrho(\tau_x A) = \varrho(A) \quad \text{for all } x \in \mathbf{Z}^v, A \in \mathfrak{A}.$$

⁷ We denote by $\mathcal{P}(E)$ the set of all subsets of E .

An interaction Φ of the lattice gas is a real function on the finite subsets of Z^v satisfying

1. $\Phi(\emptyset) = 0$,
2. translation invariance: $\Phi(X + x) = \Phi(X)$,
3. $\|\Phi\| = \sum_{X \ni 0} |\Phi(X)| < +\infty$. (3.3)

The interactions form a Banach space \mathcal{B} with respect to the norm (3.3). Let \mathcal{B}_0 consist of the finite range interactions, i.e. of the interactions Φ such that $\Phi(X) \neq 0$ for only a finite number of sets $X \ni 0$; the space \mathcal{B}_0 is dense in \mathcal{B} . For finite X , $\Lambda \subset Z^v$ we let

$$U_\Phi(X) = \sum_{Y \subset X} \Phi(Y), \tag{3.4}$$

$$P_\Lambda(\Phi) = N(\Lambda)^{-1} \log \sum_{X \subset \Lambda} \exp[-U_\Phi(X)] \tag{3.5}$$

(where $N(\Lambda)$ is the number of elements in Λ); then one can show that the following limit exists for all $\Phi \in \mathcal{B}$:

$$P(\Phi) = \lim_{\Lambda \rightarrow \infty} P_\Lambda(\Phi) \tag{3.6}$$

when Λ tends to infinity in an appropriate sense (see Appendix A). The function P is convex and continuous on \mathcal{B} .

The definition of an invariant equilibrium state corresponding to the interaction Φ is a somewhat delicate question which has been considered in detail in the literature⁸. A description of the problem is given in Appendix A, which contains also the proof of Theorem 3.2 below. Here it is convenient to accept provisionally the following somewhat untransparent definition.

3.1. Definition. If $\Psi \in \mathcal{B}$, let $A_\Psi \in \mathcal{A}$ be defined by

$$A_\Psi(X) = \sum_{Y \subset X: Y \ni 0} \frac{\Psi(Y)}{N(Y)}. \tag{3.7}$$

An invariant state ρ on \mathcal{A} is an invariant equilibrium state for the interaction Φ if the linear functional $\Psi \rightarrow -\rho(A_\Psi)$ is tangent to the graph of $P(\cdot)$ at $(\Phi, P(\Phi))$, i.e. if

$$P(\Phi + \Psi) \geq P(\Phi) - \rho(A_\Psi) \quad \text{for all } \Psi \in \mathcal{B}. \tag{3.8}$$

3.2. Theorem. For finite $\Lambda \subset Z^v$, let $f_\Lambda \in \mathcal{C}(\mathcal{P}(\Lambda) \times \mathcal{P}(Z^v \setminus \Lambda))$ be defined by

$$f_\Lambda(X, Y) = \exp \left[- \sum_{S \subset X \cup Y: S \cap X \neq \emptyset} \Phi(S) \right]. \tag{3.9}$$

⁸ See GALLAVOTTI and MIRACLE [7], RUELLE [24], LANFORD and ROBINSON [16]; for a review see RUELLE [25].

An invariant state ϱ is an invariant equilibrium state if and only if, for all A and X ,

$$\varrho_A(X, dY) = f_A(X, Y) \varrho_A(\emptyset, dY) \tag{3.10}$$

where the notation (3.2) has been used.

This theorem is proved in Appendix A. The Eqs. (3.10) can be understood as follows. Instead of an infinite system, consider a system enclosed in the finite region $M \subset \mathbb{Z}^v$. The equilibrium state of the latter system is described by a measure μ on $\mathcal{P}(M)$ such that⁹, if $X \subset M$,

$$\mu(\{X\}) = \left\{ \sum_{Y \subset M} \exp[-U_\Phi(Y)] \right\}^{-1} \exp[-U_\Phi(X)]. \tag{3.11}$$

Now, if $A \subset M$ and $X \subset A, Y \cap A = \emptyset$, we have

$$\mu(\{X \cup Y\}) = \exp \left[- \sum_{S \subset X \cup Y: S \cap X \neq \emptyset} \Phi(S) \right] \mu(\{Y\}). \tag{3.12}$$

If we formally let $M \rightarrow \infty$ in (3.12) we obtain (3.10).

It is known (see Appendix A) that for each $\Phi \in \mathcal{B}$ there is at least one invariant equilibrium state and therefore an invariant state satisfying (3.10).

3.3. Definition. A state ϱ on \mathfrak{A} is an equilibrium state for the interaction Φ if it satisfies the equations (3.10). We denote by Δ_Φ or Δ the set of equilibrium states for Φ .

By Theorem 3.2, an invariant equilibrium state is an equilibrium state, and in particular Δ is not empty; Δ is convex and compact for the weak topology¹⁰.

3.4. Theorem. A state $\varrho \in \Delta$ has short range correlations if and only if it is an extremal point of Δ .

The non-extremality of ϱ in Δ is equivalent to the existence of $h \in L^\infty(\varrho), 0 \leq h \leq 1, h$ not a multiple of 1, such that $h\varrho$ satisfies (3.10), i.e.

$$h(X, Y) \varrho_A(X, dY) = f_A(X, Y) h(\emptyset, Y) \varrho_A(\emptyset, dY). \tag{3.13}$$

Since ϱ satisfies (3.10), (3.13) is equivalent to

$$\varrho_A(X, dY) [h(X, Y) - h(\emptyset, Y)] = 0$$

i.e. to $h(X, Y) = h(\emptyset, Y)$ ϱ -almost everywhere. This means that $h \in \pi_\varrho(\tilde{\mathfrak{A}}_A)$ and therefore $h \in \mathcal{B}_{\pi_\varrho}$. But the existence of $h \in \mathcal{B}_{\pi_\varrho}, 0 \leq h \leq 1, h$ not a multiple of 1, is equivalent to ϱ not having short range correlations, proving the theorem.

The following result shows that every equilibrium state has a unique decomposition into equilibrium states with short range correlations.

⁹ This is the "grand canonical" prescription of GIBBS, with the factor $1/kT$ and the chemical potential term absorbed in the definition of the interaction Φ .

¹⁰ The weak topology of the dual of $\mathcal{C}(K)$, also called the vague topology.

3.5. Proposition. *The set Δ_ϕ is a simplex in the sense of Choquet; hence, every $\rho \in \Delta_\phi$ is the resultant of a unique measure m_ρ on Δ_ϕ carried by the extremal points of Δ_ϕ :*

$$\rho(A) = \int \sigma(A) dm_\rho(\sigma) \quad (3.14)$$

for all $A \in \mathfrak{A}$.

Let \mathfrak{B}_ϕ be the vector space of measures on K which satisfy (3.10). If $\mu \in \mathfrak{B}_\phi$, then $|\mu| \in \mathfrak{B}_\phi$; therefore, \mathfrak{B}_ϕ is a lattice¹¹ with respect to the usual order relation for measures. Since Δ_ϕ is a basis of the cone of positive elements of \mathfrak{B}_ϕ , Δ_ϕ is a simplex in the sense of Choquet¹². The fact that every $\rho \in \Delta_\phi$ has a unique integral representation in terms of extremal points of Δ_ϕ follows then from the metrizability of Δ_ϕ ¹³.

4. Non Existence of Metastable States

It is known that if water is heated above its boiling point at a certain pressure, it does not necessarily undergo the expected phase transition to water vapor but may stay in the liquid phase in a so-called *metastable state*. A great variety of such metastable states are known experimentally.

One may think that metastable states are truly unstable but, due to the finite size of systems, decay only very slowly in time¹³. Another possibility is that a metastable state for an infinite systems has an infinite lifetime and is very similar to a true equilibrium state except that it does not obey the usual variational principle (maximum entropy at fixed energy and density or maximum pressure at fixed temperature and chemical potential). In support of the second alternative comes the fact that a metastable branch occurs in the Van der Waals theory, suggesting that metastable states are in general analytic continuations of stable equilibrium states.

In this section we give a certain number of negative results, tending to prove that metastable states, as close analogues or analytic continuations of stable equilibrium states, cannot exist.

We consider the case of lattice gases¹⁴; then the proof of Theorem 3.2 (see Appendix A) gives in particular.

4.1. Proposition. *An invariant state ρ satisfying the Eqs. (3.10) and metastable in the sense that*

$$s(\rho) - \rho(A_\phi) < P(\Phi)$$

cannot exist (the entropy $s(\cdot)$ is defined by (A.9)).

¹¹ I.e. every finite set of elements of \mathfrak{B}_ϕ has a g.l.b. and a l.u.b.

¹² See CHOQUET and MEYER [2].

¹³ Slowly provided that the effect of impurities and other disturbances is adequately eliminated.

¹⁴ An extension to hard core continuous systems is immediate.

In Fig. 1 we draw a typical pressure versus activity isotherm with a kink at z_0 corresponding to a first order phase transition. We have also drawn a “metastable branch” (dotted) below the equilibrium curve. From Proposition 4.1, it follows that there cannot exist an invariant state ϱ_m satisfying the Eqs. (3.10) and corresponding to the point (z_m, P_m) .

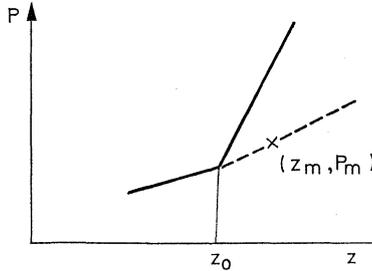


Fig. 1

4.2. Proposition. *Suppose that Φ has finite range and that P is not analytic with respect to z at z_0 . It is impossible that a state ϱ_z be defined for z in a neighborhood of z_0 so that*

1. *The correlation functions¹⁵ $\varrho_z(X)$ are real analytic in z .*
2. *ϱ_z is the stable equilibrium state for $z \leq z_0$.*

Since Φ has finite range, the Eqs. (3.10) may be written in the form (A.6) and therefore expressed in terms of the correlation functions (the $\varrho_A(\{X\})$ are finite linear combinations of the $\varrho(Y)$). The Eqs. (A.6), which are satisfied by ϱ_z for $z \leq z_0$, remain satisfied for $z > z_0$ by analytic continuation. Therefore (by Theorem 3.2) ϱ_z corresponds to a tangent of the graph of P for all z in a neighborhood of z_0 and in particular the one-point correlation function (density) is given by

$$\varrho_z(\{0\}) = z \frac{d}{dz} P(\Phi(z)).$$

The analyticity in z of the left-hand side contradicts the assumed existence of a singularity of the right-hand side at z_0 , proving the proposition.

Remark. In the same direction of excluding the existence of metastable states, it has been conjectured by FISCHER [6] that, as an analytic function of z , P must exhibit a singularity at the point z_0 of a first order phase transition; a proof of this fact has been announced for the Ising model by a group of Russian workers [1].

¹⁵ We define $\varrho(X) = \int \varrho_X(X, dY)$; see Section 5.

5. Application: Derivation of the Kirkwood-Salsburg Equations

In this section we show that one can, from the Eqs. (3.10), derive the Kirkwood-Salsburg equations for the correlation functions. Since it is known that under suitable conditions (sufficiently low activity), the Kirkwood-Salsburg equations have a unique solution¹⁶, it follows that under these conditions the set Δ_Φ of equilibrium states is reduced to a point.

We assume that Φ is a pair interaction, i.e. $\Phi(X) = 0$ if $N(X) > 2$; we may then write

$$f_\Lambda(X, Y) = z^{N(X)} \exp \left[- \sum_{\{x, x'\} \subset X} \varphi(x' - x) - \sum_{x \in X} \sum_{y \in Y} \varphi(y - x) \right] \quad (5.1)$$

where z is the activity and φ the pair potential associated with the pair interaction Φ . We have

$$D = \sum_{x \neq 0} |\varphi(x)| < +\infty. \quad (5.2)$$

We define also $\varphi(0) = +\infty$.

The correlation function associated with the state ϱ is a function $X \mapsto \varrho(X)$ of finite subsets of Z^v defined by

$$\varrho(X) = \int \varrho_X(X, dY). \quad (5.3)$$

If $x_1 \in X$ and $X_1 = X \setminus \{x_1\}$, we have

$$\begin{aligned} \varrho_X(X, dY) &= f_X(X, Y) \varrho_X(\emptyset, dY) \\ &= z \exp \left[- \sum_{x \in X_1} \varphi(x - x_1) \right] \prod_{y \in Y} [1 + (e^{-\varphi(y - x_1)} - 1)] \\ &\quad \cdot f_X(X_1, Y) \varrho_X(\emptyset, dY) \\ &= z \exp \left[- \sum_{x \in X_1} \varphi(x - x_1) \right] \sum_{S \subset Y} \prod_{y \in S} (e^{-\varphi(y - x_1)} - 1) \varrho_X(X_1, dY). \end{aligned}$$

Therefore

$$\begin{aligned} \varrho(X) &= \int \varrho_X(X, dY) \\ &= z \exp \left[- \sum_{x \in X_1} \varphi(x - x_1) \right] \int \sum_{S \subset Y} \prod_{y \in S} (e^{-\varphi(y - x_1)} - 1) \varrho_X(X_1, dY) \\ &= z \exp \left[- \sum_{x \in X_1} \varphi(x - x_1) \right] \sum_{S \subset Z^v \setminus X} \int \prod_{y \in S} (e^{-\varphi(y - x_1)} - 1) \\ &\quad \cdot \varrho_{X \cup S}(X_1 \cup S, dZ) \\ &= z \exp \left[- \sum_{x \in X_1} \varphi(x - x_1) \right] \sum_{S \subset Z^v \setminus X} \prod_{y \in S} (e^{-\varphi(y - x_1)} - 1) \\ &\quad \cdot \int \varrho_{X \cup S}(X_1 \cup S, dZ) \\ &= z \exp \left[- \sum_{x \in X_1} \varphi(x - x_1) \right] \sum_{S \subset Z^v \setminus X} \prod_{y \in S} (e^{-\varphi(y - x_1)} - 1) \\ &\quad \cdot [\varrho(X_1 \cup S) - \varrho(X \cup S)]. \end{aligned}$$

¹⁶ See RUELLE [20].

Therefore

$$\varrho(X) = z \exp \left[- \sum_{x \in X_1} \varphi(x - x_1) \right] \sum_{S \subset \mathbb{Z}^d \setminus X_1} \prod_{y \in S} (e^{-\varphi(y - x_1)} - 1) \varrho(X_1 \cup S) \quad (5.4)$$

These relations are the Kirkwood-Salsburg equations; they determine uniquely the correlation function and therefore the state ϱ if

$$z \left[\exp \sum_{x \neq 0} |\varphi(x)| \right] \left[\exp \sum_x |e^{-\varphi(x)} - 1| \right] < 1 \quad (5.5)$$

(in particular if $z < \exp[-D - e^D]$).

Instead of the Kirkwood-Salsburg equations one could obtain other equations, due to GALLAVOTTI and MIRACLE¹⁷ and for which it is not necessary to assume that Φ is a pair interaction; we write

$$f_A(X, Y) = z^{N(X)} \exp \left[- \sum_{S \subset X \cup Y: S \cap X \neq \emptyset} \Phi'(X) \right] \quad (5.6)$$

where $\Phi'(X) = 0$ when $N(X) = 1$. One finds here that the set Δ_Φ of equilibrium states is reduced to a point if

$$\frac{ze^{D-\sigma}}{1 + ze^{D-\sigma}} \cdot [2 \exp(e^D - 1) - 1] < 1 \quad (5.7)$$

where

$$C = \sum_{X \geq 0} \Phi'(X), \quad D = \sum_{X \geq 0} |\Phi'(X)| = \|\Phi'\|. \quad (5.8)$$

Using the fact that the extremal points of Δ have short range correlations (Theorem 3.4), we see that, when the correlation functions are uniquely determined by the Kirkwood-Salsburg equations or the equations of GALLAVOTTI and MIRACLE the (unique) equilibrium state has short range correlations and therefore, by Proposition 2.3 and Corollary 2.4, has strong cluster properties.

6. Time-Invariance of Equilibrium States

In this section, we give a heuristic argument indicating that states of continuous classical-mechanical systems satisfying the analogue of (3.10) should be invariant under time evolution. We proceed in the following way: Consider first a finite system in a region M , and the part of that system contained in a smaller region A . Using LIOUVILLE'S equation for the time-evolution of density distributions in M , we obtain an integrodifferential equation giving the time derivative of the density distributions in A in terms of the density distributions in a larger region A' . Since M no longer appears in this equation, we can take this system of equations as describing the time-evolution of the part of an infinite system which is contained in the bounded

¹⁷ See GALLAVOTTI and MIRACLE [8], GALLAVOTTI, MIRACLE, and ROBINSON [10] and RUEELLE [25] (Theorem 4.2.7.).

region Λ . We then show using these equations that any state which satisfies the continuous analogue of (3.10) has zero time derivative. We emphasize that the argument is only heuristic: For infinite systems in more than one dimension, no satisfactory theory of time-evolution exists, and, even for one-dimensional systems for which such a theory does exist [14], we have not shown that our formal condition for invariance under infinitesimal time translations rigorously implies time-invariance. Since our argument is only formal we will not worry about differentiability questions and interchanges of order of limits. We will assume that the finite systems we consider interact by interparticle forces defined by potentials with finite range R and with conservative external forces defining the walls of the system.

Before looking at the time-evolution problem, we outline the description of a state for an infinite continuous system in terms of local density distributions. Consider first a system in a bounded region M . The state of the system is specified by giving the density distributions $f_M^{(n)}(q_1, \dots, q_n; p_1, \dots, p_n)$ such that the probability of finding precisely n particles in M , and these particles with positions and velocities defining a point of $E \subset (M \times \mathbf{R}^v)^n$ is

$$\frac{1}{n!} \int_E dq_1 \dots dq_n dp_1 \dots dp_n f_M^{(n)}(q_1, \dots, q_n; p_1, \dots, p_n).$$

(We are using the functional notation for measures, so the formulas we write will be strictly valid only for measures absolutely continuous with respect to Lebesgue measure; it is not hard to rewrite them in a way that allows general probability measures). The function $f_M^{(n)}(q_1, \dots, q_n; p_1, \dots, p_n)$ is symmetric in the variables (q_i, p_i) and normalized by

$$\sum_{n=0}^{\infty} \frac{1}{n!} \int_{(M \times \mathbf{R}^v)^n} dq_1 \dots dq_n dp_1 \dots dp_n f_M^{(n)}(q_1, \dots, q_n; p_1, \dots, p_n) = 1. \quad (6.1)$$

If $\Lambda \subset M$, then the density distributions in Λ are given by

$$f_\Lambda^{(n)}(q_1, \dots, q_n, p_1, \dots, p_n) = \sum_{l=0}^{\infty} \frac{1}{l!} \int_{(M \setminus \Lambda \times \mathbf{R}^v)^l} dq_{n+1} \dots dq_{n+l} dp_{n+1} \dots dp_{n+l} \cdot f_M^{(n+l)}(q_1, \dots, q_{n+l}, p_1, \dots, p_{n+l}). \quad (6.2)$$

We can abbreviate the notation by letting x denote $(n; q_1, \dots, q_n; p_1, \dots, p_n)$, letting $\mathcal{X}(M)$ denote the set of all such configurations of particles in M , and letting

$$\int_{\mathcal{X}(M)} dx = \sum_{n=0}^{\infty} \frac{1}{n!} \int dq_1 \dots dq_n dp_1 \dots dp_n.$$

Then formulas (6.1) and (6.2) can be rewritten as :

$$\int_{\mathcal{X}(M)} dx f_M(x) = 1, \tag{6.1'}$$

$$f_A(x) = \int_{\mathcal{X}(M \setminus A)} dy f_M(x, y). \tag{6.2'}$$

Suppose now that we have, for every bounded open M , a non-negative symmetric function f_M on $\mathcal{X}(M)$ satisfying (6.1), and that this system of functions satisfies (6.2) for every pair A, M of bounded open sets with $A \subset M$. The system of functions then determines a state of the infinite system as defined in [23]. We will refer to f_A as the *system of local density distributions* defining the state in question.

We return to the consideration of a system contained in the bounded open set M , with time evolution defined by a Hamiltonian H . We have, by Liouville's Theorem,

$$\frac{\partial f_M(x, y, t)}{\partial t} = \sum_{i=1}^{n+l} \left[\frac{\partial H}{\partial q_i} \frac{\partial f_M}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial f_M}{\partial q_i} \right].$$

(Here, $x = (n; q_1, \dots, q_n; p_1, \dots, p_n) \in \mathcal{X}(A)$; and $y = (l; q_{n+1}, \dots, q_{n+l}; p_{n+1}, \dots, p_{n+l}) \in \mathcal{X}(M \setminus A)$). Integrating over y gives :

$$\frac{\partial f_A(x, t)}{\partial t} = \int_{\mathcal{X}(M \setminus A)} dy \sum_{i=1}^{n+l} \left[\frac{\partial H}{\partial q_i} \frac{\partial f_M}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial f_M}{\partial q_i} \right].$$

We will assume that f_M is even in each p_i separately; this will be the case, for example, if the momentum distribution is Maxwellian. (This assumption is not necessary, but it permits considerable simplifications; it implies that there is no net flow of particles into A). Then $\frac{\partial H}{\partial q_i} \frac{\partial f_M}{\partial p_i}$ and $\frac{\partial H}{\partial p_i} \frac{\partial f_M}{\partial q_i}$ are both odd in p_i , so the terms with $n+1 \leq i \leq n+l$ in the above equation give zero when integrated over y . Also, for $1 \leq i \leq n$, $\frac{\partial H(x, y)}{\partial p_i}$ does not depend on y and may therefore be taken outside the integral. Finally, if we let A' denote the set of points of M which are at a distance less than R from A , and if we use x' to denote the variables in $A' \setminus A$ and y' to denote the variables in $M \setminus A'$, then, for $1 \leq i \leq n$, $\frac{\partial H(x, x', y')}{\partial q_i}$ does not depend on y' so

$$\begin{aligned} \int_{\mathcal{X}(M \setminus A)} dy \frac{\partial H}{\partial q_i} \frac{\partial f_M}{\partial p_i} &= \int_{\mathcal{X}(A' \setminus A)} dx' \frac{\partial H(x, x')}{\partial q_i} \frac{\partial}{\partial p_i} \int_{\mathcal{X}(M \setminus A')} dy' f_M(x, x', y', t) \\ &= \int_{\mathcal{X}(A' \setminus A)} dx' \frac{\partial H(x, x')}{\partial q_i} \frac{\partial f_{A'}(x, x', t)}{\partial p_i}. \end{aligned}$$

Thus, we obtain the integro-differential equation:

$$\frac{\partial f_{\Lambda}(x, t)}{\partial t} = - \sum_{i=1}^n \frac{\partial H(x)}{\partial p_i} \frac{\partial f_{\Lambda}(x, t)}{\partial q_i} - \int_{\mathcal{X}(\Lambda' \setminus \Lambda)} dx' \frac{\partial H(x, x')}{\partial q_i} \frac{\partial f_{\Lambda'}(x, x', t)}{\partial p_i}. \quad (6.3)$$

If, now, M contains all points within a distance R of Λ , and if the external forces defining the walls of M do not affect particles inside Λ , Eq. (6.3) is independent of M and we can let $M \rightarrow \infty$. We will therefore take the system of Eqs. (6.3), with Λ running over all bounded open sets, to describe the time evolution of the state of the infinite system defined by the system of density distributions $\{f_{\Lambda}\}$.

We next show, using these equations, that an equilibrium state has zero time derivative. As above, for any bounded open set Λ , let Λ' be the set of points at a distance less than R from Λ . Let $\Lambda'' = (\Lambda')'$, let x denote a variable in $\mathcal{X}(\Lambda)$, x' a variable in $\mathcal{X}(\Lambda' \setminus \Lambda)$, and x'' a variable in $\mathcal{X}(\Lambda'' \setminus \Lambda')$. Let y be a configuration of particles in $R^{\nu} \setminus \Lambda''$, and let $W(x'', y)$ denote the energy of interaction between the configuration (x, x', x'') in Λ'' and the configuration y . We have built into our notation the fact that, because the range of the potentials is R , this interaction energy depends only on x'' and y . All we will use of the definition of equilibrium state is that an equilibrium state is defined by a system of local density distributions with $f_{\Lambda''}(x, x', x'')$ a linear superposition of functions of the form $e^{-\beta H(x, x', x'') - \beta W(x'', y)}$. It will thus suffice to prove that, if

$$f_{\Lambda', y}(x, x') = \int_{\mathcal{X}(\Lambda'' \setminus \Lambda')} dx'' e^{-\beta H(x, x', x'') - \beta W(x'', y)}$$

and if

$$f_{\Lambda, y}(x) = \int_{\mathcal{X}(\Lambda' \setminus \Lambda)} dx' f_{\Lambda', y}(x, x'),$$

then, for $1 \leq i \leq n$

$$\frac{\partial f_{\Lambda, y}(x)}{\partial q_i} \frac{\partial H(x)}{\partial p_i} = \int_{\mathcal{X}(\Lambda' \setminus \Lambda)} dx' \frac{\partial H(x, x')}{\partial q_i} \frac{\partial f_{\Lambda', y}(x, x')}{\partial p_i}.$$

This formula is proved by a straightforward calculation, which we omit.

Appendix A. Equilibrium States

Before coming to the proof of Theorem 3.2, we mention a certain number of facts connected with the definition of invariant equilibrium states.

First, when we write $\Lambda \rightarrow \infty$ for finite $\Lambda \in \mathcal{Z}^{\nu}$ we mean convergence in the sense of van Hove, i.e. $N(\Lambda) \rightarrow \infty$ and for every finite set $X \subset \mathcal{Z}^{\nu}$:

$$N(\{x : x + X \subset \Lambda\}) / N(\Lambda) \rightarrow 1.$$

If A, M are finite subsets of Z^v and $A \in \mathcal{Q}_A$, the finite system equilibrium state is given, according to (3.11) by

$$\mu_M(A) = \left\{ \sum_{X \subset M} \exp[-U_\Phi(X)] \right\}^{-1} \sum_{X \subset M} A(X) \exp[-U_\Phi(X)] \tag{A.1}$$

where we have assumed $A \subset M$. Without this assumption, we define another linear functional $\bar{\mu}_{MA}$ on \mathcal{Q}_A , obtained by averaging μ_{MA} over translations:

$$\bar{\mu}_{MA}(A) = N(M)^{-1} \sum_{x: x+A \subset M} \mu_M(\tau_x A). \tag{A.2}$$

A.1. Theorem¹⁸. *Let Γ_Φ be the set of all invariant equilibrium states for Φ . Then:*

a) *The set*

$$D = \{ \Phi \in \mathcal{B} : \Gamma_\Phi \text{ consists of a single point } \varrho^\Phi \}$$

is dense in \mathcal{B} .

b) *Let $\Phi \in \mathcal{B}$. Given a sequence $M_n \rightarrow \infty$ there exists a subsequence M'_n and $\varrho \in \Gamma_\Phi$ such that for every finite $A \subset Z^v$ and $A \in \mathcal{Q}_A$,*

$$\lim_{n \rightarrow \infty} \bar{\mu}_{M'_n A}(A) = \varrho(A). \tag{A.3}$$

In particular, if $\Phi \in D$,

$$\lim_{M \rightarrow \infty} \bar{\mu}_{MA}(A) = \varrho^\Phi(A). \tag{A.4}$$

c) *Let (Φ_i, ϱ_i) be any sequence such that $\Phi_i \in \mathcal{B}$, $\varrho_i \in \Gamma_{\Phi_i}$, $\Phi_i \rightarrow \Phi$ and (ϱ_i) has the (weak) limit ϱ ; then $\varrho \in \Gamma_\Phi$.*

d) *Let $\Phi \in \mathcal{B}$; then Γ_Φ is the closed convex hull of the set of all ϱ obtained in the manner of (c) with sequences such that $\Phi_i \in D$.*

We come now to the proof Theorem 3.2. First, let Φ be a finite range interaction ($\Phi \in \mathcal{B}_0$). There is then a finite set $Q \subset Z^v$, $Q \ni 0$, such that $X \neq \emptyset$ and $\Phi(X \cup Y) \neq 0$ imply $Y \subset X + Q$. In particular, Eq. (3.19) shows that $f_A(X, Y)$ depends on Y only through $Y \cap [A + Q]$. Let $A' \supset A + Q$, (3.12) and (A.2) yield

$$\bar{\mu}_{MA'}(\{X \cup Y\}) = f_A(X, Y) \bar{\mu}_{MA'}(\{Y\}). \tag{A.5}$$

Using part (b) of Theorem A.1 shows then that, for some state $\varrho \in \Gamma_\Phi$,

$$\varrho_{A'}(\{X \cup Y\}) = f_A(X, Y) \varrho_{A'}(Y) \tag{A.6}$$

where

$$\varrho_A(\{X\}) = \int \varrho_A(X, dY) \tag{A.7}$$

Therefore (3.10) is satisfied by ϱ . Using part (c) of the theorem and the density of \mathcal{B}_0 one concludes that the Eqs. (3.10) are satisfied by ϱ^Φ when $\Phi \in D$. Finally, using part (a) and part (d), one sees that Eqs. (3.10)

¹⁸ See GALLAVOTTI and MIRACLE [7] and RUELLE [24] for (a), (b) and (c), LANFORD and ROBINSON [16] for (d).

hold for all $\Phi \in \mathcal{B}$ and $\varrho \in \Gamma_\Phi$. This proves the first part of Theorem 3.2, namely that an invariant equilibrium state satisfies (3.10). To finish the proof, we show that every invariant state satisfying (3.10) is an invariant equilibrium state. An invariant state ϱ is an invariant equilibrium state if¹⁹

$$P(\Phi) = s(\varrho) - \varrho(A_\Phi). \tag{A.8}$$

where

$$s(\varrho) = \lim_{A \rightarrow \infty} \frac{1}{N(A)} S(\varrho_A), \tag{A.9}$$

ϱ_A is the measure on $\mathcal{P}(A)$ defined by (A.7), and

$$S(\varrho_A) = - \sum_{X \subset A} \varrho_A(\{X\}) \log \varrho_A(\{X\}). \tag{A.10}$$

Moreover, for any invariant state ϱ , $\varrho(A_\Phi) = \lim_{A \rightarrow \infty} \frac{1}{N(A)} \varrho_A(U_\Phi)$; also,

$$P_A(\Phi) = \sup \left\{ \frac{1}{N(A)} [S(\mu) - \mu(U_\Phi)]: \mu \text{ a probability measure on } \mathcal{P}(A) \right\}. \tag{A.11}$$

It will therefore suffice to prove the following assertion (which is a bit stronger than the statement of Theorem 3.2 since the requirement of translation invariance has been dropped).

If ϱ satisfies (3.10), then

$$\liminf_{A \rightarrow \infty} \frac{1}{N(A)} [S(\varrho_A) - \varrho_A(U_\Phi)] \geq P(\Phi). \tag{A.12}$$

Proof. By (3.10),

$$\varrho_A(\{X\}) = \int_{Y \subset Z^V \setminus A} f_A(X, Y) \varrho_A(\emptyset, dY)$$

and, therefore, ϱ_A may be expressed as a (generalized) convex linear combination of the probability measures $\mu_{A, Y}$ defined by

$$\mu_{A, Y}(\{X\}) = f_A(X, Y) / \left(\sum_{X \subset A} f_A(X, Y) \right).$$

Introducing:

$$W_\Phi(X, Y) = \sum_{\substack{S \subset X \cup Y \\ S \cap X \neq \emptyset \neq S \cap Y}} \Phi(S)$$

we get:

$$f_A(X, Y) = \exp[-U_\Phi(X) - W_\Phi(X, Y)]$$

¹⁹ For any invariant state σ one has

$$P(\Phi) \geq s(\sigma) - \sigma(A_\Phi).$$

Therefore, for all Ψ ,

$$P(\Phi + \Psi) \geq s(\varrho) - \varrho(A_{\Phi+\Psi}) = s(\varrho) - \varrho(A_\Phi) - \varrho(A_\Psi) = P(\Phi) - \varrho(A_\Psi),$$

so $\Psi \mapsto -\varrho(A_\Psi)$ is a tangent plane to the graph of P . See RUELLE [24].

and therefore:

$$S(\mu_{\Lambda, Y}) - \mu_{\Lambda, Y}(U_\Phi) - N(\Lambda) P_\Lambda(\Phi) = \mu_{\Lambda, Y}(W_\Phi(\cdot, Y)) + \log [\mu_{\Lambda, \Phi} e^{-W_\Phi(\cdot, Y)}] \geq -2 \sup_{\substack{X \subset \Lambda \\ Y \subset \mathbb{R}^v \setminus \Lambda}} |W_\Phi(X, Y)|.$$

By the concavity of S ,

$$\frac{1}{N(\Lambda)} [S(\varrho_\Lambda) - \varrho_\Lambda(U_\Phi)] - P_\Lambda(\Phi) \geq \frac{-2}{N(\Lambda)} \sup_{\substack{X \subset \Lambda \\ Y \subset \mathbb{R}^v \setminus \Lambda}} |W_\Phi(X, Y)|.$$

An elementary calculation, using (3.3), shows that the right-hand side of this inequality goes to zero as $\Lambda \rightarrow \infty$, so our assertion is proved.

Appendix B. Hard Core Continuous Systems

We turn now to the case of hard core continuous systems²⁰. The diameter of the hard core is a fixed number $a > 0$. We define K to be the set of subsets X of \mathbb{R}^v such that if $x, x' \in X, x \neq x'$ then $|x - x'| \geq a$ where $|\cdot|$ is the Euclidean distance. Given a bounded open set $\Lambda \subset \mathbb{R}^v$ and an integer $n \geq 0$ we define

$$O_{\Lambda n} = \{X \in K : N(X \cap \Lambda) \geq n\} \tag{B.1}$$

Similarly for a compact $F \subset \mathbb{R}^v$ we let

$$O_{Fn} = \{X \in K : N(X \cap F) \leq n\}. \tag{B.2}$$

The sets $O_{\Lambda n}$ and O_{Fn} generate a topology for which K is compact. We let $\mathfrak{A} = \mathcal{C}(K)$; for a bounded open set $\Lambda \subset \mathbb{R}^v$ we define \mathfrak{A}_Λ to be the subalgebra of \mathfrak{A} constituted by the functions which depend upon X only through $X \cap \Lambda$. The translations of \mathbb{R}^v define automorphisms τ_x of \mathfrak{A} in an obvious manner.

A state ϱ on \mathfrak{A} is a measure on K . Given a bounded open set $\Lambda \subset \mathbb{R}^v$ we write

$$\oint_\Lambda dX F(X) = \sum_n \frac{1}{n!} \int_\Lambda dx_1 \dots \int_\Lambda dx_n F(\{x_1, \dots, x_n\}) \tag{B.3}$$

where the integrations are with respect to Lebesgue measure and are restricted by $|x_j - x_i| \geq a$ if $i \neq j$. We write also, as in (3.2)²¹,

$$\varrho(\Lambda) = \oint_\Lambda dX \int A(X \cup Y) \varrho_\Lambda(X, dY). \tag{B.4}$$

²⁰ See GALLAVOTTI and MIRACLE [9].

²¹ Equation (B.4) is imprecise in two respects. First, there need not exist a function $X \mapsto \varrho_\Lambda(X, \cdot)$ from configurations in Λ to measures on the set of configurations with no particle in Λ making (B.4) true. This difficulty can easily be remedied by replacing "function" by "measure" in the obvious way; however, we shall be interested only in the case where such a function does exist. Second, even formally, the equation defines for a given X only a measure on the set of configurations Y with no particles in Λ and such that $X \cup Y \in K$. We remedy this defect by defining the measure on the set of configurations Y such that $X \cup Y \notin K$ to be zero.

Let K_n be the subspace of K consisting of sets X such that $N(X) = n$ and let K_F be the topological sum of the K_n . Let \mathcal{B}^* be the space of real continuous functions Φ on K_F satisfying

1. $\Phi(\emptyset) = 0$,
2. translation invariance: $\Phi(X + x) = \Phi(X)$.

We say that $\Phi \in \mathcal{B}^*$ is a *finite range interaction* if there exists $C_\Phi > 0$ such that $\Phi(X) = 0$ whenever the Euclidean diameter of X is larger than C_Φ . We let $\mathcal{B}_0 \subset \mathcal{B}^*$ be the space of finite range interactions. Let also \mathcal{B}^{**} be the subspace of \mathcal{B}^* constituted by those Φ such that

$$\|\Phi\| = \sup_{X \in K, X \neq \emptyset} \sum_{Y \subset X, N(Y) < +\infty} |\Phi(Y)| < +\infty. \tag{B.5}$$

Finally let \mathcal{B} be the closure of \mathcal{B}_0 in \mathcal{B}^{**} with respect to the norm (B.5). The elements of \mathcal{B} are taken as the *interactions* of hard core continuous systems.

If $X \in K_F$ we retain the definition (3.4) of U_Φ . If Λ is bounded open in \mathbf{R}^v , we define P_Λ by

$$P_\Lambda(\Phi) = V(\Lambda)^{-1} \int_\Lambda \exp[-U_\Phi(X)] dX \tag{B.6}$$

where $V(\Lambda)$ is the Lebesgue measure of Λ and the notation (B.3) has been used. We define P by (3.6) where Λ tends to infinity in the sense of van Hove, i.e. $V(\Lambda) \rightarrow \infty$ and, for all $\delta > 0$, $V(\Lambda)^{-1} V_\delta(\Lambda) \rightarrow 0$ where $V_\delta(\Lambda)$ is the Lebesgue measure of the set of points of \mathbf{R}^v with Euclidean distance to the boundary of Λ less than δ .

We choose a continuous function $\varphi \geq 0$ on \mathbf{R}^v such that $\int \varphi(x) dx = 1$ and $\varphi(x) = 0$ for $|x| > \frac{1}{2}a$. We let also $\varphi(\{x_1, \dots, x_n\}) = \sum_{i=1}^n \varphi(x_i)$ and, by analogy with (3.7) we define

$$A_\varphi(X) = \sum_{Y \subset X} \varphi(Y) \frac{\Psi(Y)}{N(Y)}. \tag{B.7}$$

With this modification we accept Definition 3.1. for an *invariant equilibrium state*. Theorem 3.2 is then replaced by the following result.

B.1. Theorem. *Let Λ be a bounded open subset of \mathbf{Z}^v ; let $X, Y \in K$, with $X \subset \Lambda$, $Y \subset \mathbf{Z}^v \setminus \Lambda$, and define*

$$f_\Lambda(X, Y) = \exp \left[- \sum_{S \subset X \cup Y; S \cap X \neq \emptyset} \Phi(S) \right] \quad \text{if } X \cup Y \in K$$

$$= 0 \quad \text{if } X \cup Y \notin K. \tag{B.8}$$

An invariant state ρ is an invariant equilibrium state if and only if, for all Λ and all $X \subset \Lambda$,

$$\rho_\Lambda(X, dY) = f_\Lambda(X, Y) \rho_\Lambda(\emptyset, dY) \tag{B.9}$$

where the notation (B.4) has been used.

The second part of the proof of Theorem 3.2 may be adapted with only minor changes in notation to apply to the case at hand. A similar modification can be carried out on the first part of the proof, using the following lemma and an analogous lemma for sequences of states on a fixed \mathfrak{A}_Λ satisfying the analogue of (A.5) for a fixed finite-range interaction.

B.2. Lemma. *Let Φ_n be a sequence in \mathcal{B} converging to Φ , and for each n let ϱ_n be a state satisfying (B.9) for the interaction Φ_n . Assume that ϱ_n converges weakly to ϱ . Then ϱ satisfies (B.9) with the interaction Φ .*

We let \mathfrak{A}_∞ denote the C^* algebra of all (bounded) Borel functions on K which are uniform limits of sequences of bounded Borel functions each of which depends on X only through $X \cap \Lambda$ for some bounded open Λ . Now (B.9) may be re-expressed in the following way: For any $A \in \mathcal{C}(K)$,

$$\begin{aligned} \varrho(A) &= \oint_A dX \int_{Y \cap \Lambda = \emptyset} f_\Lambda(X, Y) A(X \cup Y) \varrho(dY) \\ &= \int \varrho(dY) A_{\Phi, \Lambda}(Y) \end{aligned} \tag{B.10}$$

where

$$\begin{aligned} A_{\Phi, \Lambda}(Y) &= \oint_A dX f_\Lambda(X, Y) A(X \cup Y) \quad \text{if } Y \cap \Lambda = \emptyset \\ &= 0 \quad \text{if } Y \cap \Lambda \neq \emptyset. \end{aligned} \tag{B.11}$$

(In the above equations, $A(X \cup Y)$ is defined arbitrarily for $X \cup Y \notin K$). The function $A_{\Phi, \Lambda}$ is easily seen to belong to \mathfrak{A}_∞ ; moreover, $\lim_{n \rightarrow \infty} \|A_{\Phi_n, \Lambda} - A_{\Phi, \Lambda}\| = 0$ if $\Phi_n \rightarrow \Phi$ in the Banach space \mathcal{B} of interactions.

Hence, it will suffice to prove that

$$\lim_{n \rightarrow \infty} \varrho_n(B) = \varrho(B) \tag{B.12}$$

for every $B \in \mathfrak{A}_\infty$; we already know that this is true for $B \in \mathcal{C}(K)$.

Now let

$$\begin{aligned} \varrho_{n, \Lambda}(X) &= \int \varrho_{n, \Lambda}(X, dY) \\ &= \int f_A^{\Phi_n}(X, Y) \varrho_{n, \Lambda}(\emptyset, dY); \end{aligned} \tag{B.13}$$

if B is any bounded Borel function on K which depends only on $X \cap \Lambda$, we have:

$$\varrho_n(B) = \oint_A dX \varrho_{n, \Lambda}(X) B(X). \tag{B.14}$$

It is not hard to verify from the definition of the space of interactions that there is a constant C_Λ such that

$$f_A^{\Phi_n}(X, Y) \leq C_\Lambda$$

for all n , all $X \subset \Lambda$, and all $Y \subset \mathbf{Z}^r \setminus \Lambda$. Since

$$\int \varrho_{n, \Lambda}(\emptyset, dY) < 1,$$

we get

$$\varrho_{n,A}(X) < C_A \quad (\text{B.15})$$

for all n, X .

From (B.15), (B.14), and the fact that (B.12) holds for all B in \mathcal{Q}_A , it follows that (B.12) holds for all bounded Borel functions B depending only on $X \cap A$ and therefore for all $B \in \mathcal{Q}_\infty$.

From Theorem B.1, it follows that (3.3) is again a reasonable definition of an equilibrium state; with this definition, the set \mathcal{A} of equilibrium states is again convex and compact. Theorem 3.4 and Proposition 3.5 remain true, their proofs being left unchanged.

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O. E. LANFORD
Department of Mathematics
University of California
Berkeley, California, USA

D. RUELLE
Institut des Hautes
Etudes Scientifiques
F 91 Bures-sur-Yvette