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Statistical Mechanics of Quantum Spin Systems

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Abstract. The thermodynamic limit of a quantum spin system is considered. It is demonstrated that for a large class of interactions and a wide range of the thermodynamic parameters the equilibrium state of the system is describable by an extremal Z^ν-invariant state (a single phase state) over a C^* algebra of local observables. It is further shown that the equilibrium state may be obtained as the solution of a variational problem involving the mean entropy. These results extend results previously obtained for classical spin systems by GALLAVOTTI, MIRACLE-SOLE and RUELLE.

1. Introduction

In recent articles [1, 2, 3] the statistical mechanics of classical spin systems has been considered and it has been shown that, for a large class of interactions and values of the thermodynamic parameters, the state of equilibrium can be described by an extremal (single phase) Z^ν invariant state over a C^* algebra $\mathfrak{A}$ of local observables. Further it was demonstrated that the equilibrium state may be obtained as the solution of a variational problem involving the mean entropy of the Z^ν invariant states over $\mathfrak{A}$. The purpose of the present article is to derive similar results for a quantum spin system; our methods are those of [2] and [3].

2. Notation

Consider particles on a lattice Z^ν and assume that the occupation number n_i of every lattice point x_i is restricted to take the values $0, 1, \ldots, N$ where $N < +\infty$. We call such a system a spin system; this terminology originates from the fact that $\frac{1}{2}(2n_i - N)$ may be viewed as the value of a spin component.

To describe a quantum spin system we associate with each point $x_i \in Z^\nu$ a Hilbert space $\mathscr{H}_{x_i}$ of dimension $N + 1$ and with the finite set $\Lambda = \{x_1, \ldots, x_v\}$ we associate the direct product space $\mathscr{H}_\Lambda = \prod^{\otimes}_{x_i \in \Lambda} \mathscr{H}_{x_i}$. Further we define the algebra of (strictly) local observables $\mathfrak{A}(\Lambda)$ corresponding to Λ to be given by the algebra $\mathfrak{B}(\mathscr{H}_\Lambda)$ of all bounded operators acting on $\mathscr{H}_\Lambda$. Now if $\Lambda_1 \subset \Lambda_2$ an operator $A_1 \in \mathfrak{A}(\Lambda_1)$ may be identified with an operator $A_2 \in \mathfrak{A}(\Lambda_2)$ by setting $A_2 = A_1 \otimes I_{\Lambda_1/\Lambda_2}$ where I_Λ is the identity operator on $\mathscr{H}_\Lambda$ and Λ_1/Λ_2 denotes the complement of Λ_1 in Λ_2. This identification induces a norm preserving mapping $\mathfrak{A}(\Lambda_1) \to \to \mathfrak{A}(\Lambda_2)$ of the abstract C^* algebras and the isotony relationship $\mathfrak{A}(\Lambda_1) \subset \mathfrak{A}(\Lambda_2)$ for $\Lambda_1 \subset \Lambda_2$. Due to this isotony relationship, the set theoretic union of all $\mathfrak{A}(\Lambda)$ with Λ finite is a normed *algebra and we define the completion of this algebra to be the abstract C^* algebra $\mathfrak{A}$ of (quasi) local observables. We note that the group Z^ν of space translations is a subgroup of the automorphism group of $\mathfrak{A}$ and we denote the action of this group by $A \in \mathfrak{A}(\Lambda) \to \tau_x A \in \mathfrak{A}(\Lambda + x)$, $x \in Z^\nu$. Further, the subalgebras $\mathfrak{A}(\Lambda)$ satisfy the commutation relations[1]

$$[\mathfrak{A}(\Lambda_1), \mathfrak{A}(\Lambda_2)] = 0 \quad \text{if} \quad \Lambda_1 \cap \Lambda_2 = \emptyset$$

and $\mathfrak{A}$ is asymptotically Abelian, i.e.,

$$\|[A, \tau_x B]\| \xrightarrow[|x| = \infty]{} 0, \quad A, B \in \mathfrak{A}, \; x \in Z^\nu .$$

We assume that the particles on the lattice interact through many body "potentials" $\phi^{(k)}(x_0, \ldots, x_{k-1}) \in \mathfrak{A}(\{x_0, \ldots, x_{k-1}\})$. We consider an interaction ϕ to be a sequence $\phi = (\phi^{(k)})_{k \geqq 1}$ of k body "potentials" which we assume to have the properties

I. $\phi^{(k)}(x_0, \ldots, x_{k-1})$ is Hermitian

II. $\phi^{(k)}(x_0 + x, \ldots, x_{k-1} + x) = \tau_x \phi^{(k)}(x_0, \ldots, x_{k-1}), \quad x \in Z^\nu$

and

III. $$\|\phi\| = \sum_{k \geqq 1} \frac{1}{k!} \sum_{x_1, \ldots, x_{k-1} \in Z^\nu}^{\neq 0} \|\phi^{(k)}(0, x_1, \ldots, x_{k-1})\| < +\infty$$

where the sum $\sum^{\neq 0}$ extends over all sequences of distinct points of Z^ν different from 0. The interactions ϕ form a real Banach space $\mathscr{B}$ with respect to this norm. We denote by $\mathscr{B}_0$ the dense subset $\mathscr{B}_0 \subset \mathscr{B}$ of finite range interactions, i.e., those $\phi = (\phi^{(k)})_{k \geq 1}$ for which

$$\phi^{(k)}(0, x_1, \ldots, x_{k-1}) = 0$$

unless $\{x_1, \ldots, x_{k-1}\} \subset \Lambda$ for some finite Λ.

Next, for each $\phi \in \mathscr{B}$, let us define $A_\phi \in \mathfrak{A}$ by

$$A_\phi = \sum_{k \geqq 1} \frac{1}{k!} \sum_{x_1, \ldots x_{k-1} \in Z^\nu}^{\neq 0} \phi^{(k)}(0, x_1, \ldots, x_{k-1})$$

(A_ϕ is the "interaction energy" at the origin). The mapping $\phi \to A_\phi$ is

[1] For simplicity we have omitted consideration of spin systems with anti-commutation relations (Fermi lattice gases, see [4]) but we remark that even such systems can be described in terms of observables with commutation relations. For such a description one would, however, choose $\mathfrak{A}(\Lambda)$ to be a subalgebra of $\mathfrak{B}(\mathscr{H}_\Lambda)$.

norm decreasing from $\mathscr{B}$ to $\mathfrak{A}$ and the set $\{\tau_x A_\phi; x \in Z^\nu, \phi \in \mathscr{B}_0\}$ is dense in $\mathfrak{A}$; if $\phi \in \mathscr{B}_0$ then A_ϕ is strictly local. These facts will be of significance later.

We will start by considering a system of particles on the finite set Λ and the energy operator $U_\phi(\Lambda)$ on $\mathscr{H}_\Lambda$ corresponding to the interaction ϕ will be given by

$$U_\phi(\Lambda) = \sum_{k \leqq 1} \frac{1}{k!} \sum_{x_0, \ldots, x_{k-1} \in \Lambda}^{\neq} \phi^{(k)}(x_0, \ldots, x_{k-1}).$$

We will be interested in studying functions $Z_\Lambda(\phi)$, $F_\Lambda(\phi)$ and $P_\Lambda(\phi)$ which we define as follows;

$$Z_\Lambda(\phi) = \mathrm{Tr}_{\mathscr{H}_\Lambda}(e^{-U_\phi(\Lambda)})$$

$$F_\Lambda(\phi) = \log Z_\Lambda(\phi) \quad \text{and} \quad P_\Lambda(\phi) = V(\Lambda)^{-1} F_\Lambda(\phi)$$

where $V(\Lambda)$ denotes the number of points of Λ.

3. Thermodynamic Limit

a) The Thermodynamic Free Energy

Our immediate aim is to show how the methods of [2, 3] may be used to define the thermodynamic free energy of a quantum spin system. We begin by recalling that if A and B are $n \times n$ Hermitian matrices then the following inequalities are valid [see for example [5], Eqs. (1), (2) and (19)]

$$|\log \mathrm{Tr}(e^{-A}) - \log \mathrm{Tr}(e^{-B})| \leqq \|A - B\| \tag{1}$$

and for $0 \leqq \lambda \leqq 1$

$$\log \mathrm{Tr}(e^{-\lambda A - (1-\lambda) B}) \leqq \lambda \log \mathrm{Tr}(e^{-A}) + (1-\lambda) \log \mathrm{Tr}(e^{-B}) . \tag{2}$$

These inequalities immediately yield

Lemma I. a. *If Λ_1 and Λ_2 are disjoint the function $\Lambda \to F_\Lambda(\phi)$ satisfies*

$$|F_{\Lambda_1 \cup \Lambda_2}(\phi) - F_{\Lambda_1}(\phi) - F_{\Lambda_2}(\phi)| \leqq \|U_\phi(\Lambda_1 \cup \Lambda_2) - U_\phi(\Lambda_1) - U_\phi(\Lambda_2)\| .$$

b. *The function $\phi \to P_\Lambda(\phi)$ is convex and continuous on $\mathscr{B}$; for $\phi, \psi \in \mathscr{B}$ and $1 \geqq \lambda \geqq 0$*

$$P_\Lambda(\lambda\phi + (1-\lambda)\psi) \leqq \lambda P_\Lambda(\phi) + (1-\lambda) P_\Lambda(\psi)$$

and, further

$$|P_\Lambda(\phi) - P_\Lambda(\psi)| \leqq \|\phi - \psi\| . \tag{3}$$

Proof. The first statement of the Lemma follows from (1) if we choose $A = U_\phi(\Lambda_1 \cup \Lambda_2)$ and $B = U_\phi(\Lambda_1) + U_\phi(\Lambda_2)$ and note that as Λ_1 and Λ_2 are disjoint

$$\mathrm{Tr}_{\mathscr{H}_{\Lambda_1 \cup \Lambda_2}}(e^{-U_\phi(\Lambda_1) - U_\phi(\Lambda_2)}) = \mathrm{Tr}_{\mathscr{H}_{\Phi_1}}(e^{-U_\phi(\Lambda_1)}) \, \mathrm{Tr}_{\mathscr{H}_{\Lambda_2}}(e^{-U_\phi(\Lambda_2)}) .$$

The convexity of $P_\Lambda(\phi)$ follows directly from (2) if we choose $A = U_\phi(\Lambda)$, $B = U_\psi(\Lambda)$ whilst (3) is a consequence of (1) and the inequality

$$\|U_\phi(\Lambda) - U_\psi(\Lambda)\| = \|U_{\phi-\psi}(\Lambda)\| \leqq V(\Lambda)\|\phi - \psi\| .$$

From this Lemma, we may conclude the following:

Theorem I. *If $\phi \in \mathscr{B}$ then the limit*

$$P(\phi) = \lim_{\Lambda \to \infty} \frac{1}{V(\Lambda)} F_\Lambda(\phi) = \lim_{\Lambda \to \infty} P_\Lambda(\phi)$$

exists, where Λ tends to infinity in the sense of Van Hove (see [1]). The function $\phi \to P(\phi)$ is convex and continuous on the Banach space $\mathscr{B}$ and

$$|P(\phi) - P(\psi)| \leqq \|\phi - \psi\| .$$

The proof of this theorem is obtained by combining the arguments of [2] and [5]; we refer to these papers for details. The first stage in the proof is to conclude the existence of $P(\phi)$ for $\phi \in \mathscr{B}_0$; this is discussed in [5] for the case of Λ being a parallelepiped with sides tending to infinity. The extension of the arguments of [5] to the more general type of limit is easy. The second stage (see [2]) is to note that if the sequence $\phi_n \in \mathscr{B}_0$ tends to ϕ, i.e., if $\|\phi_n - \phi\| \xrightarrow[n=\infty]{} 0$ then $P_\Lambda(\phi_n)$ tends to $P_\Lambda(\phi)$ uniformly in Λ as a result of (3). This is sufficient to establish the existence of the limit $P(\phi)$. The convexity and continuity of $\phi \to P(\phi)$ follow immediately from the Lemma.

The connection between this theorem and the thermodynamics of the spin system is given by introducing the inverse temperature β and defining $\Xi_\Lambda(\beta, \phi)$ through

$$\Xi_\Lambda(\beta,\phi) = Z_\Lambda(\beta\phi) .$$

Then $\Xi_\Lambda(\beta, \phi)$ is interpretable as the partition function of the set Λ and the above theorem establishes the existence of the thermodynamic free energy

$$p(\beta, \phi) = \beta^{-1} P(\beta\phi) = \beta^{-1} \lim_{\Lambda\to\infty} \frac{1}{V(\Lambda)} \log \Xi_\Lambda(\beta, \phi).$$

Other parameters than β, such as the components of an external magnetic field, may also be introduced through the interaction ϕ. Bounds on $p(\beta, \phi)$ may be easily obtained from (3).

b) *The Equilibrium State*

Let Λ' be a subsystem of a spin system confined to Λ. For $A \in \mathfrak{A}(\Lambda')$ define $\varrho_{\phi,\Lambda}(A)$ by

$$\varrho_{\phi,\Lambda}(A) = \frac{1}{Z_\Lambda(\phi)} \mathrm{Tr}_{\mathscr{H}_\Lambda}(e^{-U_\phi(\Lambda)} A) .$$

The expectation values $\varrho_{\phi,\Lambda}(A)$ give information concerning the physical properties of the subsystem Λ'. If the size of Λ is increased then physically the effects of the boundary of Λ should in many circumstances become negligible in Λ'; mathematically this would be reflected by the $\varrho_{\phi,\Lambda}$ tending to a limit ϱ_ϕ as $\Lambda \to \infty$. The resulting limit function ϱ_ϕ would then determine a state over $\mathfrak{A}$. We next consider the existence of such a limit state.

Notice that if ϱ_ϕ exists it will be a Z^ν invariant state due to the assumed invariance of ϕ. This indicates another procedure for examining the limit. If $\psi \in \mathscr{B}_0$ then A_ψ is strictly local and $\varrho_\phi(A_\psi)$ would give the "energy" at the origin due to the interaction ψ. However, due to the invariance this "energy" would also be equal to the "average energy" due to ψ. Thus it would be expected that $\varrho_\phi(A_\psi)$ should also exists as the limit of the expectation value of the "average energy" $V(\Lambda)^{-1}\, U_\psi(\Lambda)$. We therefore consider the expectation values, $\alpha_{\phi,\Lambda}(\psi)$, of the average energies defined by

$$\alpha_{\phi,\Lambda}(\psi) = \varrho_{\phi,\Lambda}\left(\frac{U_\psi(\Lambda)}{V(\Lambda)}\right) = \frac{1}{V(\Lambda)}\,\frac{1}{Z_\Lambda(\phi)}\,\mathrm{Tr}_{\mathscr{H}_\Lambda}(e^{-U_\phi(\Lambda)}\,U_\psi(\Lambda))\,.$$

The above heuristic discussion is partially justified by showing that as $\Lambda \to \infty$ the sequence $\alpha_{\phi,\Lambda}(\psi)$ converges to a limit $\alpha_\phi(\psi)$. Finally, in Section 5, we will prove the existence of a state ϱ_ϕ over $\mathfrak{A}$ which is such that $\varrho_\phi(A_\psi) = \alpha_\phi(\psi)$.

The following theorem is due to Gallavotti and Miracle-Sole.

Theorem II. *Let $T \subset \mathscr{B}$ be the set of ϕ such that the graph of $P(\phi)$ has a unique tangent plane at ϕ, i.e., there exists a unique α_ϕ in the dual $\mathscr{B}^*$ of $\mathscr{B}$ such that for all $\psi \in \mathscr{B}$*

$$P(\phi + \psi) \geqq P(\phi) - \alpha_\phi(\psi)$$

then for $\phi \in T$ and $\psi \in \mathscr{B}$

$$\alpha_\phi(\psi) = \lim_{\Lambda\to\infty} \alpha_{\phi,\Lambda}(\psi) = \lim_{\Lambda\to\infty} \frac{1}{V(\Lambda)}\,\frac{1}{Z_\Lambda(\phi)}\,\mathrm{Tr}_{\mathscr{H}_\Lambda}(e^{-U_\phi(\Lambda)}\,U_\psi(\Lambda))$$

where the limit $\Lambda \to \infty$ is in the sense of Van Hove.

The proof of the theorem is identical to that of [2] once one notes that for finite Λ the function $\phi \to P_\Lambda(\phi)$ has a unique tangent plane namely $\alpha_{\phi,\Lambda}$. We omit the details.

As $\phi \to P(\phi)$ is a convex function one may obtain rather good characterizations of the set T for which the above limits exist (see [2]). For example one may deduce that for a dense set of interactions $\phi \in \mathscr{B}$

$$\alpha_{\beta\phi}(\psi) = \lim_{\Lambda\to\infty} \alpha_{\beta\phi,\Lambda}(\psi)$$

for almost all β. We have postponed to Section 5 the completion of the argument of the existence of the equilibrium state ϱ_ϕ. We will also show that when ϱ_ϕ can be defined as a limit of the type considered in the theorem then ϱ_ϕ describes physically a single thermodynamic phase. Thus the exceptional points for which the limits do not exist correspond in the physical interpretation to the points for which the coexistence of phases is possible. Thus for a large class of interactions the state of equilibrium is a single phase situation for almost all temperatures.

Note that although we have aimed at introducing a Z^ν invariant state to describe equilibrium this does not rule out the possibility of spontaneous symmetry breakdown.

4. Mean Entropy

a) Definition

Our next aim is to describe how one may associate an entropy per site, or mean entropy, to each Z^ν invariant state of the quantum spin system. Discussions of the mean entropy in quantum statistical mechanics are given in [4] and [6].

Each state ϱ over the algebra $\mathfrak{A}$ is locally describable by a density matrix $\varrho_\Lambda \in \mathfrak{A}(\Lambda)$, i.e.,

$$\varrho(A) = \mathrm{Tr}_{\mathscr{H}_\Lambda}(\varrho_\Lambda A), \quad A \in \mathfrak{A}(\Lambda).$$

The family $\{\varrho_\Lambda\}$ of density matrices has the properties

$$\text{I} \qquad \mathrm{Tr}_{\mathscr{H}_\Lambda}(\varrho_\Lambda) = 1$$

and

$$\text{II} \qquad \mathrm{Tr}_{\mathscr{H}_{\Lambda_1}}(\varrho_{\Lambda_1 \cup \Lambda_2}) = \varrho_{\Lambda_2} \quad \text{if,} \quad \Lambda_1 \cap \Lambda_2 = \theta.$$

Introducing an entropy $S_\varrho(\Lambda)$ by

$$S_\varrho(\Lambda) = -\mathrm{Tr}_{\mathscr{H}_\Lambda}(\varrho_\Lambda \log \varrho_\Lambda)$$

we may conclude [4] that

$$0 \leqq S_\varrho(\Lambda) \leqq V(\Lambda)\log(N+1) \tag{4}$$

$$S_\varrho(\Lambda_1 \cup \Lambda_2) \leqq S_\varrho(\Lambda_1) + S_\varrho(\Lambda_2) \quad \text{if} \quad \Lambda_1 \cap \Lambda_2 = \theta. \tag{5}$$

Now let us consider invariant states. We will need to consider not only Z^ν invariant states but also certain periodic states, i.e., states invariant under a subgroup of Z^ν. We do not need to study the most general periodic state but, for each integer n, we define the set K_n by

$$K_n = \{\varrho \in E; \varrho(A) = \varrho(\tau_{na}A), A \in \mathfrak{A}, a \in Z^\nu\}$$

(E is the set of all states over $\mathfrak{A}$.) The invariance property implies that for each $\varrho \in K_n$ there exist unitaries U_ϱ which relate the density matrices via

$$\text{III} \qquad \varrho_{\Lambda+na} = U_\varrho(na)\varrho_\Lambda U_\varrho(na)^{-1}, \quad a \in Z^\nu.$$

If for $a = (a_1, \ldots, a_\nu) \in Z^\nu$, $a_1 > 0, \ldots, a_\nu > 0$ we let

$$\Lambda(na) = \{x \in Z^\nu; 0 \leqq x_i < na_i, i = 1, \ldots \nu\}$$

then we may prove the following:

Theorem III. *The mean entropy $S_n(\varrho)$,*

$$S_n(\varrho) = \lim_{a_1,\ldots a_\nu \to \infty} \frac{S(\Lambda(na))}{V(\Lambda(na))} = \inf_{a_1,\ldots a_\nu} \frac{S(\Lambda(na))}{V(\Lambda(na))},$$

exists and the function $\varrho \to S_n(\varrho)$ is affine, upper semi-continuous, with respect to the W^* topology, on K_n; $S_n(\varrho) \in [0, \log(N+1)]$. Further we *have*

$$\lim_{a_1,\ldots a_\nu\to\infty} \frac{S_\varrho(\Lambda(na)+b)}{V(\Lambda(na))} = \lim_{a_1\ldots a_\nu\to\infty} \frac{S_\varrho(\Lambda(na))}{V(\Lambda(na))}, \; b\in Z^\nu$$

A proof of all but the last statement of the theorem is given in [4]. Let us consider the last statement. Without loss of generality we may assume $0 < b_i < n$ and then, writing $e = (1, \ldots, 1) \in Z^\nu$, we have from (4) and (5)

$$S_\varrho(\Lambda(na)+b) \leqq S_o\big(\Lambda(n(a-e))+ne\big) + V(\Lambda_{na}^{n(a-e)})\log(N+1)$$

and

$$S_\varrho(\Lambda(na)+b) \geqq S_\varrho\big(\Lambda(n(a+e))\big) - V(\Lambda_{n(a+e)}^{na})\log(N+1)$$

where we have used Λ_b^a to denote the complement of $\Lambda(a)$ in $\Lambda(b)$. Dividing these inequalities by $V(\Lambda(na))$ and taking the appropriate limit yields the desired results.

Next let us remark that we may associate with each state $\tilde\varrho\in K_n$ an averaged state $\varrho\in K_1$ by the definition

$$\varrho = \frac{1}{n^\nu}\sum_{x\in\Lambda(ne)} \tau'_x\tilde\varrho \tag{6}$$

where

$$(\tau'_x\tilde\varrho)(A) = \tilde\varrho(\tau_x A)\,.$$

The above theorem immediately implies the following

Corollary. *The entropies $S_1(\varrho)$ and $S_n(\tilde\varrho)$ are equal.*

Proof. We have

$$S_1(\varrho) = S_n\left(\frac{1}{n^\nu}\sum_{x\in\Lambda(ne)}\tau'_x\tilde\varrho\right) = \frac{1}{n^\nu}\sum_{x\in\Lambda(ne)} S_n(\tau'_x\tilde\varrho) = S_n(\tilde\varrho)$$

where we have used the affine property of S_n, and the last statement of the theorem namely $S_n(\tau'_x\tilde\varrho) = S_n(\tilde\varrho)$, $x\in Z^\nu$.

This result will be used in the next Section.

b) Variational Property

The results of the foregoing Sections now allow us to reproduce the results obtained in [3] for classical spin systems

Theorem IV. *If $\phi\in\mathscr{B}$ then we have*

$$P(\phi) = \sup_{\varrho\in K_1}\,[S_1(\varrho) - \varrho(A_\phi)]\,.$$

Proof. The proof is similar to that in [3] and proceeds in two steps. First we show that for $\varrho\in K_1$

$$P(\phi) \geqq S_1(\varrho) - \varrho(A_\phi) \tag{7}$$

and secondly we exhibit a $\varrho \in K_1$ with the property that

$$P(\phi) < S_1(\varrho) - \varrho(A_\phi) + \varepsilon \,. \tag{8}$$

Given $\varepsilon > 0$ we may choose Λ sufficiently large that

$$\left\| \frac{1}{V(\Lambda)} \sum_{x \in \Lambda} \tau_x A_\phi - \frac{1}{V(\Lambda)} U_\phi(\Lambda) \right\| < \varepsilon$$

and hence

$$\left| \varrho(A_\phi) - \frac{1}{V(\Lambda)} \mathrm{Tr}(\varrho_\Lambda U_\phi(\Lambda)) \right| < \varepsilon \,.$$

But

$$S_1(\varrho) \leqq - \frac{1}{V(\Lambda)} \mathrm{Tr}(\varrho_\Lambda \log \varrho_\Lambda) \,.$$

Thus

$$S_1(\varrho) - \varrho(A_\phi) - \varepsilon < - \frac{1}{V(\Lambda)} \mathrm{Tr}(\varrho_\Lambda \log \varrho_\Lambda + \varrho_\Lambda U_\phi(\Lambda)) \,.$$

Now if ψ_i is a complete orthonormal set of eigenfunctions of ϱ_Λ with corresponding eigenvalues ϱ_i $(0 \leqq \varrho_i \leqq 1, \sum_i \varrho_i = 1)$ then

$$\begin{aligned} S_1(\varrho) - \varrho(A_\phi) - \varepsilon &< \frac{1}{V(\Lambda)} \sum_i \varrho_i \log \frac{e^{-(\psi_i, U_\phi(\Lambda)\psi_i)}}{\varrho_i} \\ &\leqq \frac{1}{(V\Lambda)} \log \sum_i e^{-(\psi_i, U_\phi(\Lambda)\psi_i)} \\ &\leqq P(\phi) \end{aligned} \tag{9}$$

where the first step is a consequence of the convexity of the logarithm and the second step is an application of a theorem due to PEIERLS, namely

$$\sum_i e^{-(\psi_i, U_\phi(\Lambda)\psi_i)} \leqq \mathrm{Tr}(e^{-U_\phi(\Lambda)}) \,.$$

(For a rigorous demonstration, due to JOST, of this theorem, see [7].) Taking the limit $\Lambda \to \infty$ in (9) gives (7).

Next we construct a state $\tilde{\varrho} \in K_n$ by giving the following prescription for the family of density matrices $\{\tilde{\varrho}_\Lambda\}$. The sets $\Lambda_n^a = \Lambda(ne) + na$ with $a \in Z^\nu$ form a partition $\mathscr{P}_n$ of Z^ν. Define

$$\tilde{\varrho}_{\Lambda_n^a} = \frac{1}{Z_{\Lambda_n^a}(\phi)} e^{-U_\phi(\Lambda_n^a)}$$

and

$$\tilde{\varrho}_{\Lambda_n^A} = \prod_{a \in A}^{\otimes} \tilde{\varrho}_{\Lambda_n^a} \quad \text{for} \quad \Lambda_n^A = \bigcup_{a \in A} \Lambda_n^a \tag{10}$$

where A is any finite subset of Z^ν. These density matrices are sufficient to define the state $\tilde{\varrho} \in K_n$. If we then construct an invariant state $\varrho \in K_1$ by the procedure (6) the corollary to Theorem III tells us that

$$S_1(\varrho) = S_n(\tilde{\varrho}) \,.$$

However, as $\tilde{\varrho}$ has the product structure (10) we find immediately

$$\begin{aligned} S_1(\varrho) = S_n(\tilde{\varrho}) &= -\frac{1}{V(\Lambda(ne))} \operatorname{Tr}\left(\tilde{\varrho}_{\Lambda(ne)} \log \tilde{\varrho}_{\Lambda(ne)}\right) \\ &= \frac{1}{V(\Lambda(ne))} \operatorname{Tr}\left(\tilde{\varrho}_{\Lambda(ne)} U_\phi(\Lambda(ne))\right) + P_{\Lambda(ne)}(\phi) . \end{aligned} \tag{11}$$

But, noting that

$$\varrho(A_\phi) = \frac{1}{V(\Lambda(ne))} \tilde{\varrho}\Big(\sum_{x \in \Lambda(ne)} \tau_x A_\phi\Big)$$

it is easily seen that for each $\varepsilon > 0$ one can choose n large enough that both

$$\left|\varrho(A_\phi) - \frac{1}{V(\Lambda(ne))} \tilde{\varrho}\big(U_\phi(\Lambda(ne))\big)\right| < \frac{\varepsilon}{2} \tag{12}$$

and

$$|P(\phi) - P_{\Lambda(ne)}(\phi)| < \frac{\varepsilon}{2} . \tag{13}$$

Combining (11), (12) and (13) yields (8) and concludes the proof of the theorem.

The above theorem may now be used to complete the discussion of the equilibrium state which was begun in Section 3b.

5. The Equilibrium State

We have shown that

$$P(\phi) = \sup_{\varrho \in K_1} [S_1(\varrho) - \varrho(A_\phi)] . \tag{14}$$

Assuming that the supremum is attained for $\varrho = \varrho_\phi \in K$, then we immediately have that for $\psi \in \mathscr{B}$

$$P(\phi + \psi) \geqq S_1(\varrho_\phi) - \varrho_\phi(A_{\phi+\psi}) = P(\phi) - \varrho_\phi(A_\psi) .$$

Thus, since $\psi \to A_\psi$ is linear and continuous, the function $\psi \to \varrho_\phi(A_\psi)$ is a tangent plane to the graph of $P(\cdot)$ at ϕ. Now if we can deduce that different states which yield the supremum in (14) also give distinct tangent planes we may deduce that for $\phi \in T$ the supremum is reached at exactly one point $\varrho_\phi \in K_1$ and, due to the affine character of the function $\varrho \to S_1(\varrho) - \varrho(A_\phi)$, this state must be an extremal point of K_1. This final deduction is, however, immediately given by replacing $\mathfrak{C}(K)$ in the proof given by Ruelle [3] (cf. Theorem IV) for the classical case, by $\mathfrak{A}$. Ruelle's proof does not depend on the Abelian character of $\mathfrak{C}(K)$. Further, as $\mathfrak{A}$ is asymptotically Abelian, an extremal invariant state can be shown to correspond to a single thermodynamic phase using results obtained earlier [8, 9].

Formally, we may summarize the above statements together with those of Section 3b as follows:

Theorem V. *If* $\phi \in T$ *the function* $\varrho \to S_1(\varrho) - \varrho(A_\phi)$ *reaches its maximum at exactly one point* $\varrho_\phi \in K_1$ *and, further, if* α_ϕ *is the tangent plane to* $P(.)$ *at* ϕ *then for all* $\psi \in \mathscr{B}$

$$\varrho_\phi(A_\psi) = \alpha_\phi(\psi) = \lim_{\Lambda \to \infty} \frac{1}{V(\Lambda)} \frac{1}{Z_\Lambda(\phi)} \mathrm{Tr}_{\mathscr{H}_\Lambda}(e^{-U_\phi(\Lambda)} U_\psi(\Lambda)) .$$

Finally, for $\phi \in T$, *the "equilibrium state"* ϱ_ϕ *is an extremal point of* K_1 *and hence describes a single thermodynamic phase.*

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