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# Statistical Mechanics of Quantum Mechanical Particles with Hard Cores

## II. The Equilibrium States

SALVADOR MIRACLE-SOLE
C.N.R.S., Marseille

DEREK W. ROBINSON
Centre Universitaire, Luminy, Marseille

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**Abstract.** The states of a quantum mechanical system of hard core particles are characterized as a convex weak * compact subset of the states over a $C^*$ algebra associated with the canonical (anti-) commutation relations. It is shown that the mean conditional entropy, i.e. entropy minus energy, can be defined as an affine upper semi-continuous function over the $G$-invariant hard core states where $G$ is an invariance group containing space translations. An abstract definition of the pressure and equilibrium states is given in terms of the maximum of the conditional entropy and it is shown that the pressure $P_S$ obtained in this way satisfies $P \geqq P_S \geqq P_\infty$ where $P$ and $P_\infty$ are the thermodynamic pressures obtained from the usual Gibbs formalism with elastic wall, and repulsive wall, boundary conditions respectively. A number of additional results concerning the equilibrium states are also given.

## 1. Introduction

This paper is a continuation of [11] which we will refer to as I. The purpose of these papers is to attempt to extend results obtained in [1–7] [1] to the more general setting of quantum hard core systems. In this second paper we consider the properties of the equilibrium states and show that most of the results of [1–7] can indeed be generalized. The one feature we have not been able to establish is true if the two pressures $P$ and $P_\infty$ introduced in I are equal; thus in effect we reduce the whole problem to this one point, the equality of $P$ and $P_\infty$.

## 2. Observables and Hard Core States

We will consider particles satisfying Bose-Einstein statistics and leave the easier discussion of Fermi particles to the reader.

[1] We number the references of this paper consecutively with those of I, i.e. Refs. [1–10] should be sought in I.

The states of a system of Bose point particles can be described by the states over various $C^*$ algebras associated with the canonical commutation relations. We will consider two such algebras which we introduce as follows. Let $\Lambda$ be an open bounded subset of $R^\nu$ and let $L^2_+(\Lambda^n)$ denote the Hilbert space of totally symmetric square integrable functions of $n$ points in $\Lambda$. Define the Fock space $\mathscr{H}(\Lambda)$ by

$$\mathscr{H}(\Lambda) = \bigoplus_{n \geqq 0} L^2_+(\Lambda^n),$$

i.e. an element of $\mathscr{H}(\Lambda)$ is a sequence $\Psi = (\Psi^{(n)})_{n \geqq 0}$ where $\Psi^{(0)}$ is a complex scalar, $\Psi^{(n)} \in L^2_+(\Lambda^n)$ for $n \geqq 1$, and the scalar product is defined by:

$$(\Psi, \Phi) = \int_\Lambda dX\, \overline{\Psi(X)}\, \Phi(X)$$

where we use the set theoretic notation

$$\Psi(X) = \Psi(x_1, \ldots, x_n) \quad \text{if} \quad X = \{x_1, \ldots, x_n\}$$

and

$$\int_\Lambda dX \cdot = \sum_{n \geqq 0} \int_{\Lambda^n} \frac{dx_1 \ldots dx_n}{n!} \cdot$$

For each real $f, g \in L^2(\Lambda)$ we can introduce by a standard definition unitary operators $U(f)$, $V(g)$ on $\mathscr{H}(\Lambda)$ satisfying the Weyl form of the canonical commutation relations:

$$U(f)\, V(g) = V(g)\, U(f)\, e^{i(f \cdot g)} \quad \text{etc.}$$

Finally we introduce two local algebras of observables $\mathfrak{A}(\Lambda)$ and $\mathfrak{L}(\Lambda)$ associated with this structure. $\mathfrak{A}(\Lambda)$ is defined to be he smallest $C^*$ algebra, acting on $\mathscr{H}(\Lambda)$, which contains $\{U(f), V(g); f, g \in L^2(\Lambda)\}$ and $\mathfrak{L}(\Lambda)$ is defined to be the $C^*$ algebra of all bounded operators on $\mathscr{H}(\Lambda)$. The algebras $\mathfrak{A}$ and $\mathfrak{L}$ of quasi-local observables are then defined in a standard manner to be the norm closures of the families $\{\mathfrak{A}(\Lambda); \Lambda \subset R^\nu\}$ and $\{\mathfrak{L}(\Lambda); \Lambda \subset R^\nu\}$ respectively.

Next we describe the states of a system of bosons with hard cores of diameter $a$ contained in $\Lambda$. The set $F_a^\Lambda$ of physical configurations is defined by

$$F_a^\Lambda = \{X; X \subset \Lambda, |x_i - x_j| \geqq a \text{ for } x_i, x_j \in X \text{ and } i \neq j\}.$$

Note that the number of points in the set $X$ takes values $0, 1, \ldots, N_a(\Lambda)$. We introduce $\varrho_a$ by the definition

$$\varrho_a = \lim_{\Lambda \to R^\nu} \frac{N_a(\Lambda)}{V(\Lambda)}$$

and the limit is taken over the net of increasing parallepipeds where $V(\Lambda)$ denotes the volume, i.e. Lebesgue measure, of $\Lambda$. The Hilbert space $\mathscr{H}_a(\Lambda)$ of the finite system of hard core particles is defined by

$$\mathscr{H}_a(\Lambda) = \{\Psi; \Psi \in \mathscr{H}(\Lambda), \tilde{\Psi}(X) = 0 \text{ if } X \not\subset F_a^\Lambda\}$$

with the scalar product the same as that of $\mathscr{H}(\Lambda)$. The space $\mathscr{H}_a(\Lambda)$ is a closed subspace of $\mathscr{H}(\Lambda)$ and we denote by $P_a^\Lambda$ the associated orthogonal projection operator. Note that $P_a^\Lambda \in \mathfrak{L}(\Lambda)$.

We next give a definition of hard core states as states over the quasi-local algebra $\mathfrak{A}$. Recall that a state $\varrho$ over $\mathfrak{A}$ is said to be locally normal if the restriction of $\varrho$ to each $\mathfrak{A}(\Lambda)$ is normal, i.e. if $\varrho$ restricted to each $\mathfrak{A}(\Lambda)$ is determined by a density matrix $\varrho_\Lambda$ on $\mathscr{H}(\Lambda)$.

**Definition 1.** *The set $\mathscr{V}$ of hard core states over the algebra $\mathfrak{A}$ is defined to be the subset of locally normal states $\varrho$ whose corresponding density matrices $\varrho_\Lambda$ satisfy*

$$\varrho_\Lambda = \varrho_\Lambda P_a^\Lambda (= P_a^\Lambda \varrho_\Lambda = P_a^\Lambda \varrho_\Lambda P_a^\Lambda)$$

*for all open bounded $\Lambda \subset R^\nu$.*

The following properties of the $\mathscr{V}$ are of use.

**Theorem 1.** *The set $\mathscr{V}$ of hard core states is convex and compact in the weak* topology induced by $\mathfrak{A}$.*

*Proof.* $\mathscr{V}$ is clearly convex. We will prove the compactness property by using a set $\mathscr{W}$ of states over $\mathfrak{L}$ which we define to be the set of states $\varrho$ with the property that $\varrho(P_a^\Lambda) = 1$ for all $\Lambda \subset R^\nu$. It is clear that $\mathscr{W}$ is weak* compact (with respect to the dual topology of $\mathfrak{L}$) because the conditions $\varrho(P_a^\Lambda) = 1$ define weak* closed sets of states. Further we have that $\mathscr{W} \mid \mathfrak{A}$ is weak* compact (with respect to the dual topology of $\mathfrak{A}$) because the restriction procedure is a continuous mapping and the image of a compact set under a continuous mapping is compact. Further if $\varrho \in \mathscr{V}$ then the ultraweakly continuous extensions of $\varrho$ over the $\mathfrak{A}(\Lambda)$ to states over $\mathfrak{L}(\Lambda)$ determines a state in $\mathscr{W}$. Thus $\mathscr{W} \mid \mathfrak{A} \supseteq \mathscr{V}$. We complete the proof by demonstrating that $\mathscr{V} \supseteq \mathscr{W} \mid \mathfrak{A}$.

Note that if $\varrho \in \mathscr{W}$ then the Schwartz inequality yields

$$\varrho(B) = \varrho(P_a^\Lambda B) = \varrho(B P_a^\Lambda) = \varrho(P_a^\Lambda B P_a^\Lambda), \qquad B \in \mathfrak{L}(\Lambda).$$

Using this equality we deduce from Proposition 4.1.6 of [12] [2] that $\varrho$ is a regular state over $\mathfrak{A}(\Lambda)$ and then from Theorem 4 of [12] it follows that

[2] It should be noted that the algebra $\mathfrak{C}(\Lambda)$ associated with the canonical commutation relations in [12] differs from both the algebras we consider. However, one has $\mathfrak{L}(\Lambda) \supset \mathfrak{C}(\Lambda) \supset \mathfrak{A}(\Lambda)$.

$\varrho \mid \mathfrak{A}(\Lambda)$ is normal (with the notation of [12] we can use the equality

$$\varrho(e^{iN(M)t}) = \varrho(P_a^\Lambda e^{iN(M)t} P_a^\Lambda)$$

to deduce that this latter expression is a finite polynomial in $e^{it}$ and hence the uniformity of the convergence required by criterion (d) of the above cited Theorem 4 is immediate). Finally it is straightforward to argue that the density matrix which determines the restriction of $\varrho$ to $\mathfrak{A}(\Lambda)$ must satisfy the condition $\varrho_\Lambda = \varrho_\Lambda P_a^\Lambda$ on Fock space. Hence $\mathscr{W} \mid \mathfrak{A} = \mathscr{V}$ and the proof is complete.

Next we wish to consider hard core states invariant under a group $G$ of automorphisms of $\mathfrak{A}$. There are a number of groups of interest; the group $R^\nu$ of space translations, the group $E^\nu$ of Euclidean transformations, or the product of either of these groups with the compact group of gauge transformations. The main property that all these groups have in common which allows us to proceed without a particular specification is that they are all represented as groups of automorphisms of the algebras $\mathfrak{A}$ and $\mathfrak{L}$ and both these algebras have an asymptotically abelian property with respect to each of the groups. In the following we assume that $G$ is identified with one of the above groups. We denote by $E_G$ the convex weak*-$\mathfrak{A}$ compact set of all $G$-invariant states over $\mathfrak{A}$ and by $\mathscr{E}(K)$ the extremal points of a set $K$.

**Theorem 2.** *Let $\varrho \in E_G \cap \mathscr{V}$ be a $G$-invariant hard core state over $\mathfrak{A}$. There exists a unique probability measure $\mu_\varrho$, with barycentre $\varrho$, concentred on $\mathscr{E}(E_G) \cap \mathscr{V}$ i.e. $E_G \cap \mathscr{V}$ is a Choquet simplex and there is a unique decomposition*

$$\varrho = \int_{\mathscr{E}(E_G) \cap \mathscr{V}} d\mu_\varrho(\varrho')\varrho'$$

*of $\varrho$ into extremal $G$-invariant hard core states.*

*Proof*. Firstly $\varrho$ can be extended in a unique manner to be a locally normal $G$-invariant state over $\mathfrak{L}$ and it follows from [13] that $\varrho$ has a unique barycentric decomposition into extremal $G$-invariant locally normal states $\varrho'$ over $\mathfrak{L}$. Secondly note that $\varrho(1 - P_a^\Lambda) = 0$ for all $\Lambda \subset R^\nu$ and hence $\varrho'(1 - P_a^\Lambda) = 0$ up to a set of $\mu_\varrho$-measure zero. These conditions for a denumerable set of $\Lambda$ ensure that $\mu_\varrho$ is concentrated on extremal $G$-invariant locally normal states $\varrho'$ over $\mathfrak{L}$ whose density matrices satisfy $\varrho'_\Lambda = \varrho'_\Lambda P_a^\Lambda$ for all $\Lambda \subset R^\nu$. Finally the result follows by restriction to $\mathfrak{A}$; note that the restriction, to $\mathfrak{A}$, of an extremal $G$-invariant state over $\mathfrak{L}$ is an extremal $G$-invariant state over $\mathfrak{A}$ (cf. for example the characterizations of extremal $G$-invariant states by cluster properties given in [13–15]).

## 3. Mean Energy and Conditional Entropy

We first introduce a class of local Hamiltonians which are related to those studied in I but we will characterize the interactions in terms of elements of the algebra $\mathfrak{L}$.

The hermitian elements of the algebra $\mathfrak{L}$ form a Banach space; we introduce a second Banach space $\mathscr{B}$ which is the restriction of the first space by the hard core conditions. First introduce the set $\{P_a^\Lambda B P_a^\Lambda;\ B = B^* \in \mathfrak{L}(\Lambda), \Lambda \subset R^\nu\}$ and define $\mathscr{B}_0$ to be the closure of this set through multiplications by a real scalar and addition. The space $\mathscr{B}$ is then defined as the closure of $\mathscr{B}_0$ with respect to the norm $|||.|||$, defined by

$$|||B|||^2 = \sup_{\varrho \in \mathscr{V}} \varrho(B^* B) \qquad B \in \mathfrak{L}$$

where the supremum is taken only over the hard core states and we use the extension:

$$\varrho(B) = \mathrm{Tr}_{\mathscr{H}_a(\Lambda)}(\varrho_\Lambda B) \qquad \varrho \in \mathscr{V}, \ B \in \mathfrak{L}(\Lambda).$$

Note that $|||B||| \leqq \|B\|$. If the invariance groups $G$ contains the group of spatial rotations or the group of gauge transformation we further restrict $B$ to contain only elements invariant under the action of these compact group of automorphisms. If $B \in \mathscr{B}_0$ we can assume that there is a $\Lambda_B$ such that $B$ is an hermitian element of $P_a^{\Lambda_B} \mathfrak{L}(\Lambda_B) P_a^{\Lambda_B}$. Now for $\Lambda \supset \Lambda_B$ introduce $U_\Lambda(B)$ by

$$U_\Lambda(B) = \int_{\Lambda_B + x \subset \Lambda} dx \, \tau_x B$$

where $x \to \tau_x$ denotes the action of the group of space translations as automorphisms of $\mathfrak{L}$. It is easily established that $U_\Lambda$ satisfies the conditions of an interaction Hamiltonian assumed in I and in particular for $\Lambda_1 \cap \Lambda_2 = \emptyset$ one finds that

$$\|U_{\Lambda_1 \cup \Lambda_2}(B) - U_{\Lambda_1}(B) - U_{\Lambda_2}(B)\| \leqq (S(\Lambda_1) + S(\Lambda_2) - S(\Lambda_1 \cup \Lambda_2)) \|B\| \, d(B)$$

where $S(\Lambda)$ denotes the surface area of $\Lambda$ and $d(B)$ is the diameter of $\Lambda_B$. Now for each such interaction and each real $\mu$ we define a total Hamiltonian $H_\Lambda(\mu, B)$ on $\mathscr{H}_a(\Lambda)$ by

$$H_\Lambda(\mu, B) = T_\Lambda^0 + U_\Lambda(B) - \mu N_\Lambda,$$

where $T_\Lambda^0$ is the self-adjoint kinetic energy operator corresponding to elastic boundary conditions and $N_\Lambda$ is the bounded number operator; these latter operators are defined in I where the definition of $H_\Lambda(\mu, B)$ is discussed at length. In particular it is established in I that $H_\Lambda(\mu, B)$ is self-adjoint with compact resolvent and in fact $\exp\{-\beta H_\Lambda(\mu, B)\}$ is of trace-class for all $\beta > 0$. Let the spectral resolution of $H_\Lambda(\mu, B)$ be given by

$$H_\Lambda(\mu, B) = \int dE(\lambda) \lambda$$

then we can define a functional over the hard core states $\mathscr{V}$ by

$$H_A(\varrho;\mu,B)=\sup_m \mathrm{Tr}_{\mathscr{H}_a(A)}\Big(\varrho_A \int_{\lambda\leqq m} dE(\lambda)\lambda\Big)$$

where $\varrho\in\mathscr{V}$ and $\varrho_A$ is the associated density matrix. It is straightforwardly checked that

$$H_A(\varrho;\mu,B)=\mathrm{Tr}_{\mathscr{H}_a(A)}(H_A^{\frac{1}{2}}(\mu,B)\,\varrho_A H_A^{\frac{1}{2}}(\mu,B))$$

whenever the operator occurring is of trace class and $H_A(\varrho;\mu,B)=+\infty$ in the other case.

Using the methods of I and [18, 17] one finds the following result.

**Lemma 1.** *For $B\in\mathscr{B}_0$ and $\mu\in R$ the function $\varrho\in\mathscr{V}\to H_A(\varrho;\mu,B)$ is affine and lower semi-continuous in the weak*-$\mathfrak{A}$ topology. It satisfies the continuity relation*

$$|H_A(\varrho;\mu,B_1)-H_A(\varrho;\mu,B_2)|\leqq V(A)\,|||B_1-B_2|||$$

*for $\varrho\in\mathscr{V}$ and $B_1,B_2\in\mathscr{B}_0$.*

*For fixed $\varrho\in\mathscr{V}$, $B\in\mathscr{B}_0$ and $\mu\in R$ one has:*

$$H_A(\varrho;\mu,B)\geqq V(A)\,\|B\|-N_a(A)\mu_M\,,$$

*where $\mu_M=\max(0,\mu)$ and if $A_1\cap A_2=\emptyset$ one has:*

$$\begin{aligned}H_{A_1\cup A_2}(\varrho;\mu,B)\geqq{}& H_{A_1}(\varrho;\mu,B)+H_{A_2}(\varrho;\mu,B)\\&-(S(A_1)+S(A_2)-S(A_1\cup A_2))\,\|B\|\,d(B)\,.\end{aligned}$$

*Proof.* The function is affine by definition and is lower semi-continuous in the weak*-$\mathfrak{A}$ topology by Theorem 3 of [17]. The continuity relation follows from the identity

$$H_A(\varrho;\mu,B_1)-H_A(\varrho;\mu,B_2)=\int_{A_B{}^+\setminus\subset A} dx\,\mathrm{Tr}_{\mathscr{H}_a(A)}(\varrho_A\tau_x(B_1-B_2))$$

The lower bound is straight forwardly derived using the facts that $T_A^0\geqq 0$ and $N_a(A)\geqq N_A\geqq 0$. The sub-additivity property follows from the argument used to prove Theorem 2 of I and is a direct consequence of the inequalities derived for the forms determined by the Hamiltonian operators.

Next introduce the parallelepiped $A_a$ by the definition

$$A_a=\{X;X\subset R^\nu,0<x_i\leqq a_i,i=1,\ldots,\nu\}$$

and recall that $G$ is assumed to contain $R^\nu$.

**Theorem 3.** *For each $\varrho\in E_G\cap\mathscr{V}$, $\mu\in R$ and $B\in\mathscr{B}_0$ the following limit*

$$H(\varrho;\mu,B)=\lim_{a_1,\ldots,a_\nu\to\infty}\frac{H_{A_a}(\varrho;\mu,B)}{V(A_a)}$$

*exists and has the property that*

$$|H(\varrho;\mu,B_1)-H(\varrho;\mu,B_2)|\leqq |||B_1-B_2||| \qquad B_1,B_2\in\mathscr{B}_0\,.$$

*Thus $H(\varrho;\mu,\cdot)$ can be extended by continuity to $\mathscr{B}$. For fixed $\mu\in R$ and $B\in\mathscr{B}$ the function $\varrho\in E_G\cap\mathscr{V}\to H(\varrho;\mu,B)$ is affine and lower semi-continuous in the weak*-$\mathfrak{A}$ topology.*

*Proof*. From the last inequality of Lemma 1 and the invariance of $\varrho$ under $R^\nu$ one finds that the function

$$a_1,\ldots,a_\nu\to H_{\Lambda_a}(\varrho;\mu,B)-S(\Lambda_a)\,\|B\|\,d(B)$$

is super-additive in each of the variables $a_i$. Further if $a_i\geqq 1$, $i=1,\ldots,\nu$ then there is a constant $C$, independent of $a_i$, such that

$$H_{\Lambda_a}(\varrho;\mu,B)-S(\Lambda_a)\,\|B\|\,d(B)\geqq C\,V(\Lambda_a)\,.$$

It then follows from a standard argument concerning super-additive functions that

$$\begin{aligned}\sup_{a_1,\ldots,a_\nu}&\frac{H_{\Lambda_a}(\varrho;\mu,B)-S(\Lambda_a)\,\|B\|\,d(B)}{V(\Lambda_a)}\\&=\lim_{a_1,\ldots,a_\nu\to\infty}\frac{H_{\Lambda_a}(\varrho;\mu,B)-S(\Lambda_a)\,\|B\|\,d(B)}{V(\Lambda_a)}\\&=\lim_{a_1,\ldots,a_\nu\to\infty}\frac{H_{\Lambda_a}(\varrho;\mu,B)}{V(\Lambda_a)}\end{aligned}$$

The existence of the limit is thus established. The continuity for $B\in\mathscr{B}_0$, then follows from Lemma 1. For $B\in\mathscr{B}_0$ the function $\varrho\to H(\varrho;\mu,B)$ is affine because it is the limit of a family of affine functions and is lower semi-continuous in the weak*-$\mathfrak{A}$ topology because we have established that it is defined as the supremum of a family of lower semi-continuous functions. The continuous extension of $H$ to $\mathscr{B}$ does not destroy these properties.

The function $\varrho\in E_G\cap\mathscr{V}\to H(\varrho;\mu,B)$ corresponds to the energy per unit volume of hard core particles with chemical potential $\mu$ and interaction density $B$ in a $G$-invariant state. We have defined this function by using the local Hamiltonian corresponding to perfectly elastic walls. Alternatively we could have used Hamiltonians corresponding to different degrees of elasticity. Thus in the above definitions we could have substituted the kinetic energy operator $T_\Lambda^\sigma$ of I for $T_\Lambda^0$ and thus defined a family of local energy functionals $H_\Lambda^\sigma(\varrho;\mu,B)$. However it would then follow from the estimate of Lemma 1 of I that

$$|H_\Lambda^\sigma(\varrho;\mu,B)-H_\Lambda^0(\varrho;\mu,B)|\leqq|\sigma|\,\varrho_a S(\Lambda)$$

and hence for $\varrho \in E_G \cap \mathscr{V}$

$$H(\varrho;\mu,B)=\lim_{a_1,\ldots,a_\nu\to\infty}\frac{H^\sigma_{\Lambda_a}(\varrho;\mu,B)}{V(\Lambda_a)}.$$

Thus the energy per unit volume is to a large extent independent of the boundary conditions used in its definition. An exception is given if one repeats the above definitions with the Hamiltonian defined in I, which corresponds to infinitely repulsive walls for the finite system. This form of boundary condition is essentially incompatible with the $R^\nu$-invariance and the only $R^\nu$-invariant state for which the corresponding local energy is not infinite is the Fock vacuum.

We next examine the entropy and conditional entropy of hard core states. Given a locally normal state $\varrho$ over $\mathfrak{A}$ we define a family of local entropies in the manner of [18] by

$$S_\Lambda(\varrho)=+\infty$$

if $\varrho_\Lambda \log \varrho_\Lambda$ is not of trace-class on $\mathscr{H}(\Lambda)$

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

otherwise, where $\{\varrho_\Lambda\}$ is the family of density matrices determining $\varrho$. In particular, we can assign local entropies to each $\varrho\in\mathscr{V}$. Theorem 1 of [18] establishes that the function $\Lambda\to S_\Lambda(\varrho)$ is positive, sub-additive and for $0<\lambda<1$:

$$0\leqq S_\Lambda(\lambda\varrho_1+(1-\lambda)\varrho_2)-\lambda S_\Lambda(\varrho_1)-(1-\lambda)\,S_\Lambda(\varrho_2)\leqq \log 2\,.$$

Further it is established in [16] and [17] that for $\varrho\in\mathscr{V}$, $\mu\in R$ and $B\in\mathscr{B}_0$

$$S_\Lambda(\varrho)\leqq \beta H_\Lambda(\varrho;\mu,B)+\log \mathrm{Tr}_{\mathscr{H}_a(\Lambda)}(e^{-\beta H_\Lambda(\mu,B)}),\qquad \beta>0\,.$$

We introduce the local conditional entropy as a function over $\mathscr{V}$ by the definition

$$S_\Lambda(\varrho;\beta,\mu,B)=S_\Lambda(\varrho)-\beta H_\Lambda(\varrho;\mu,B)$$

if $H_\Lambda(\varrho;\mu,B)<+\infty$ and by

$$S_\Lambda(\varrho;\beta,\mu,B)=-\infty$$

otherwise. In these definitions and in the following, we always take $\beta>0$, $\mu\in R$ and $B\in\mathscr{B}_0$. A slight modification of the proof of Theorem 5 of [17] establishes that the function $\varrho\in\mathscr{V}\to S_\Lambda(\varrho;\beta,\mu,B)$ is upper semi-continuous in the weak*-$\mathfrak{A}$ topology.

**Theorem 4.** *For each $\varrho\in E_G\cap\mathscr{V}$, $\beta>0$, $\mu\in R$ and $B\in\mathscr{B}_0$ the following limit:*

$$S(\varrho;\beta,\mu,B)=\mathop{\mathrm{Lim}}_{a_1,\ldots,a_\nu\to\infty}\frac{S_{\Lambda_a}(\varrho;\beta,\mu,B)}{V(\Lambda_a)}$$

*exists and has the property that*

$$|S(\varrho; \beta, \mu, B_1) - S(\varrho; \beta, \mu, B_2)| \leqq \beta|||B_1 - B_2||| \qquad B_1 B_2 \in \mathscr{B}_0 .$$

*thus* $S(\varrho; \beta, \mu, B)$ *can be extended by continuity to* $\mathscr{B}$. *For fixed* $\beta, \mu, B$ *the function* $\varrho \in E_G \cap \mathscr{V} \to S(\varrho; \beta, \mu, B)$ *is affine and upper semi-continuous in the weak*-*$\mathfrak{A}$ *topology.*

*Proof*. The theorem follows directly from the information collected above. The upper-additive property of $H_\Lambda$ established in Lemma 1, the sub-additive of $S_\Lambda$, and the definition of the conditional entropy, show that the function

$$a_1, \ldots, a_\nu \to S_{\Lambda_a}(\varrho; \beta, \mu, B) - \beta S(\Lambda_a) \, \|B\| \, d(B) .$$

is sub-additive in each variable $a_i$ whenever the hard core state $\varrho$ is $R^\nu$-invariant. However the bound on $S_\Lambda$ given above and the estimate given in Theorem 1 of I show that there is a $C$, independent of $a_1, \ldots, a_\nu$, such that

$$S_{\Lambda_a}(\varrho; \beta, \mu, B) - \beta S(\Lambda_a) \, \|B\| \, d(B) \leqq C V(\Lambda_a)$$

and thus the theorem concerning sub-additive functions establishes that

$$\begin{aligned} \inf_{a_1, \ldots, a_\nu} & \frac{S_{\Lambda_a}(\varrho; \beta, \mu, B) - \beta S(\Lambda_a) \, \|B\| \, d(B)}{V(\Lambda_a)} \\ &= \lim_{a_1, \ldots, a_\nu \to \infty} \frac{S_{\Lambda_a}(\varrho; \beta, \mu, B) - S(\Lambda_a) \, \|B\| \, d(B)}{V(\Lambda_a)} \\ &= \lim_{a_1, \ldots, a_\nu \to \infty} \frac{S_{\Lambda_a}(\varrho; \beta, \mu, B)}{V(\Lambda_a)} \end{aligned}$$

The existence of the limit is thus established for $\beta > 0$, $\mu \in R$ and $B \in \mathscr{B}_0$. The continuity for $B \in \mathscr{B}_0$ follows from the similar property for $H$.

The affinity of $\varrho \in E_G \cap \mathscr{V} \to S(\varrho; \beta, \mu, B)$ follows from the convexity property of $S_\Lambda$ and the affinity of $H_\Lambda$ and the upper semi-continuity follows because we have established that $S(.; \beta, \mu, B)$ is expressed as the lower envelope of a family of upper semi-continuous functions. Both the foregoing properties are thus valid for $B \in \mathscr{B}_0$ but they are unchanged by continuous extension from $\mathscr{B}_0$ to $\mathscr{B}$.

**Corollary 1.** *For each* $\beta > 0$, $\mu \in R$ *and* $B \in \mathscr{B}$ *the function*

$$\varrho \in E_G \cap \mathscr{V} \to S(\varrho; \beta, \mu, B)$$

*respects the barycentric decomposition of Theorem 2, i.e.*

$$S(\varrho; \beta, \mu, B) = \int_{\mathscr{E}(E_G) \cap \mathscr{V}} d\mu_\varrho(\varrho') \, S(\varrho'; \beta, \mu, B) .$$

This last property is an immediate consequence of the affinity and semi-continuity of the conditional entropy given above.

## 4. The Pressure and Equilibrium States

Using the material of the foregoing sections we can introduce the thermodynamic pressure and the set of equilibrium states for an infinite hard core system in the following abstract manner.

**Definition 2.** *The thermodynamic pressure $P_S$ is defined as a function over $R_+ \times R \times \mathscr{B}$ by*

$$P_S(\beta, \mu, B) = \sup_{\varrho \in E_G \cap \mathscr{V}} S(\varrho; \beta, \mu, B)$$

*The corresponding set $\Delta(\beta, \mu, B)$ of G-invariant equilibrium states is defined to be the set of states for which the above supremum is attained, i.e.*

$$\Delta(\beta, \mu, B) = \{\varrho; \varrho \in E_G \cap \mathscr{V}, \ P_S(\beta, \mu, B) = S(\varrho; \beta, \mu, B)\}.$$

In these definitions $\beta$ is to be physically interpreted as the inverse temperature, $\mu$ the chemical potential, and $B$ the interaction energy density. Note that the definitions are unchanged by the transformation $B \to \tau_x B$, $x \in R^\nu$. Thus we could consider the above concepts to be defined on classes of elements of $B$ formed by elements which are translates of one another, or averages of such translates; this redundancy is however unimportant in the sequel.

Although it is interesting to have a direct definition of the above physical quantities for an infinite system it is nevertheless essential that one should establish that these definitions agree with those usually given by the limit of a finite system.

We have already noted that for each $B \in \mathscr{B}$ the interaction $U_\Lambda(B)$ satisfies the conditions of an interaction Hamiltonian assumed in I and thus we can define $P$ by

$$P(\beta, \mu, B) = \operatorname*{Lim}_{a_1, \ldots, a_\nu \to \infty} \frac{1}{V(\Lambda_a)} \log \operatorname{Tr}_{\mathscr{H}_a(\Lambda_a)}(e^{-\beta H_{\Lambda_a}(\mu, B)}).$$

Similarly we could define a pressure $P_\infty$ by using the kinetic energy operator $T_\Lambda$, corresponding to "infinitely repulsive walls", in place of $T_\Lambda^0$. It is established in I that these functions are convex and continuous in $\beta$ and $\mu$ and using Proposition A 3 of I one finds that:

$$|P(\beta, \mu, B_1) - P(\beta, \mu, B_2)| \leqq \beta |||B_1 - B_2|||,$$

$$|P_\infty(\beta, \mu, B_1) - P_\infty(\beta, \mu, B_2)| \leqq \beta |||B_1 - B_2|||$$

for all $B_1, B_2 \in \mathscr{B}_0$. Thus $P$ and $P_\infty$ can be extended by continuity to functions over $R_+ \times R \times \mathscr{B}$ and we have from I that these functions are convex.

**Theorem 5.** *$P_S$ is convex, continuous in $\beta$ and $\mu$, and satisfies*

1. $|P_S(\beta, \mu, B_1) - P_S(\beta, \mu, B_2)| \leqq \beta |||B_1 - B_2|||$,
2. $P_\infty \leqq P_S \leqq P$.

*Proof*. The convexity of $P_S$ follows immediately from its definition as a supremum and the continuity in $\beta$ and $\mu$ is a consequence. But

$$\begin{aligned} P_S(\beta, \mu, B_1) &= \sup_{\varrho \in E_G \cap \mathscr{V}} [S(\varrho; \beta, \mu, B_2) + \beta\varrho(B_2 - B_1)] \\ &\leqq \sup_{\varrho \in E_G \cap \mathscr{V}} S(\varrho; \beta, \mu, B_2) + \sup_{\varrho \in E_G \cap \mathscr{V}} \varrho(B_2 - B_1) \\ &\leqq P_S(\beta, \mu, B_2) + \beta |||B_2 - B_1||| . \end{aligned}$$

This inequality and the similar one obtained by interchanging $B_1$ and $B_2$, give Property 1.

The principal result of the theorem is Property 2. The right hand equality follows from the inequality for $S_\Lambda$ given in the previous section; one has:

$$\begin{aligned} S(\varrho; \beta, \mu, B) &= \lim_{\Lambda \to \infty} \frac{S_\Lambda(\varrho; \beta, \mu, B)}{V(\Lambda)} \\ &\leqq \lim_{\Lambda \to \infty} \frac{1}{V(\Lambda)} \log \operatorname{Tr}_{\mathscr{H}_a(\Lambda)}(e^{-\beta H_\Lambda(\mu, B)}) \\ &= P(\beta, \mu, B) \end{aligned}$$

for all $\varrho \in E_G \cap \mathscr{V}$ and $B \in \mathscr{B}_0$. The desired result follows immediately.

The left hand inequality can now be deduced by construction of an invariant state $\varrho_\infty$ for which

$$S(\varrho_\infty; \beta, \mu, B) = P_\infty(\beta, \mu, B) .$$

First note that if $H_\Lambda$ denotes the Hamiltonian corresponding to the region $\Lambda$ chemical potential $\mu$, interaction $B \in \mathscr{B}_0$ and *infinitely repulsive boundary conditions* than for $\varepsilon > 0$ we can choose a parallelepiped $\Lambda_l$ such that

$$\frac{1}{V(\Lambda_l)} \log \operatorname{Tr}_{\mathscr{H}_a(\Lambda_l)}(e^{-\beta H_{\Lambda_l}}) > P_\infty(\beta, \mu, B) - \frac{\varepsilon}{2} .$$

Further using Proposition A3 of I and the definition of $H_\Lambda$ by a quadratic form we can choose a finite orthonormal family of vectors $\Psi_1, \ldots, \Psi_n \in \mathscr{H}_a(\Lambda_l)$ such that $X \in F_a^{\Lambda_l} \to \Psi_i(X)$ is infinitely often differentiable with compact support in $F_a^{\Lambda_l}$ and

$$\begin{aligned} \frac{1}{V(\Lambda_l)} \log \sum_{i=1}^{n} \exp\{-\beta \|H_{\Lambda_l}^{\frac{1}{2}} \Psi_i\|^2\} &> \frac{1}{V(\Lambda_l)} \log \operatorname{Tr}_{\mathscr{H}_a(\Lambda_l)}(e^{-\beta H_{\Lambda_l}}) - \frac{\varepsilon}{2} \\ &> P_\infty(\beta, \mu, B) - \varepsilon . \end{aligned}$$

Next define $E_i$ to be the projector with range $\Psi_i$ and introduce $\varrho_{\Lambda_l}$ to be the density matrix on $\mathscr{H}_a(\Lambda_l)$ given by

$$\varrho_{\Lambda_l} = \sum_{i=1}^{n} \exp\{-\beta \|H_{\Lambda_l}^{\frac{1}{2}} \Psi_i\|^2\} E_i / Z_{\Lambda_l}$$

where

$$Z_{\Lambda_l} = \sum_{i=1}^{n} \exp\{-\beta \| H_{\Lambda_l}^{\frac{1}{2}} \Psi_i \|^2\} .$$

Now if $\varrho_l$ denotes the normal state over $\mathfrak{A}(\Lambda_l)$ defined by the density matrix $\varrho_{\Lambda_l}$ then one straightforwardly computes that

$$S_{\Lambda_l}(\varrho_l; \beta, \mu, B) = \log Z_{\Lambda_l}$$

and hence

$$\frac{1}{V(\Lambda_l)} S_{\Lambda_l}(\varrho_l; \beta, \mu, B) > P_\infty(\beta, \mu, B) - \varepsilon .$$

Finally we use the above choice of $\varrho_{\Lambda_l}$ to construct a $G$-invariant state over $\mathfrak{A}$ by the following standard procedure. Let $n_1, \dots, n_\nu$ be integers and $\Lambda_{n,l}$ the parallelepiped centred at $(n_1(l_1+a), \dots, n_\nu(l_\nu+a))$ with edges of length $l_1 \dots l_\nu$. For each choice of $n$ we can introduce a density matrix $\varrho_{\Lambda_{n,l}}$ on $\mathscr{H}_a(\Lambda_{n,l})$ in the same manner that we introduced $\varrho_{\Lambda_l}$ above. Now let $I$ be a cubic subset of $Z^\nu$ and define

$$\Lambda_I = \bigcup_{n \in I} \Lambda_{n,l} .$$

Now on $\mathscr{H}_a(\Lambda_I)$, which is given explicitly by

$$\mathscr{H}_a(\Lambda_I) = \prod_{n \in I}^{\otimes} \mathscr{H}_a(\Lambda_{n,l}) ,$$

we define the density matrix

$$\varrho_{\Lambda_I} = \prod_{n \in I}^{\otimes} \varrho_{\Lambda_{n,l}} .$$

If $\Psi_I^i$ denote the vector states associated with $\varrho_{\Lambda_I}$ then $\varrho_{\Lambda_I}$ can be extended to be a density matrix on the Hilbert space $\mathscr{H}_a(\tilde{\Lambda}_I)$, where $\tilde{\Lambda}_I$ denotes the convex closure of $\Lambda_I$, by extending the $\Psi_I^i$ through the definition

$$\Psi_I^i(X) = 0 \quad \text{if} \quad X \in F_a^{\tilde{\Lambda}_I} \quad \text{but} \quad X \notin F_a^{\Lambda_I} .$$

It is important to realize that the choice of the density matrices $\varrho_{\Lambda_{n,l}}$ is made such that this extension is continuous and in fact $X \in F_a^{\tilde{\Lambda}_I} \to \Psi_I^i(X)$ is infinitely often differentiable with compact support. The foregoing specification for all $I$ determines a hard core state $\varrho_l$ over $\mathfrak{A}$ which is invariant under translations which are of the form $(n_1(l_1+a), \dots, n_\nu(l_\nu+a))$. Defining $\tau_x \varrho_l$ by

$$(\tau_x \varrho_l)(A) = \varrho_l(\tau_x A) \qquad A \in \mathfrak{A}$$

we can introduce an $R^\nu$-invariant hard core state by

$$\tilde{\varrho}_l = \frac{1}{V} \int' dX \, \tau_x \varrho_l$$

where the prime denotes that the integration is taken over the set $|x_i| < (l_i + a)/2$ and

$$V = \prod_{i=1}^{\nu} \left( \frac{l_i + a}{2} \right).$$

Now with this construction it can be checked that

$$S(\tilde{\varrho}_l; \beta, \mu, B) = \frac{1}{V(\Lambda_l)} S_{\Lambda_l}(\varrho_l; \beta, \mu, B) > P_\infty(\beta, \mu, B) - \varepsilon .$$

If $G$ contains the groups of space rotations and gauge transformations we can average $\tilde{\varrho}_l$ over these groups and the last estimate remains valid for the ensuring $G$-invariant state. Thus we conclude that $P_S \geqq P_\infty$.

Note that in the above construction of a $G$-invariant state it was essential to use the Hamiltonian corresponding to infinitely repulsive boundary conditions in the construction of the local density matrix $\varrho_{\Lambda_l}$. If one attempts the same construction using $H_\Lambda(\mu, B)$, i.e. elastic boundary conditions, then the $\Psi_l^i$ would be discontinuous and one would find $H(\tilde{\varrho}_l; \beta, \mu, B) = +\infty$ and consequently $S(\tilde{\varrho}_l; \beta, \mu, B) = -\infty$. Thus this construction does not seem useful to demonstrate that $P_S$ attains its upper bound $P$.

Our failure to demonstrate that $P_S = P$, or $P_S = P_\infty$, does not allow us to give such a complete discussion of the equilibrium states as has been obtained for example for quantum spin systems in [4] and [6] but a number of the advantageous properties are a consequence of the convexity and continuity properties that we have derived.

**Theorem 6.** *The sets $\Delta(\beta, \mu, B)$ of $G$-invariant equilibrium states have the following properties*

1. *$\Delta(\beta, \mu, B)$ is convex, compact in the weak*-$\mathfrak{A}$ topology, and a simplex in the sense of Choquet with the property that*

$$\mathscr{E}(\Delta(\beta, \mu, B)) \subset \mathscr{E}(E_G) \cap \mathscr{V} .$$

2. *The weak, weak*-$\mathfrak{A}$, and the locally uniform topologies induced on $(\Delta(\beta, \mu, B)$ coincide and the set is metrizable in this common topology*[3].

3. *If $\varrho \in \Delta(\beta, \mu, B)$ then*

$$P_S(\beta_1, \mu_1, B_1) \geqq P_S(\beta, \mu, B) + (\beta - \beta_1) \, H\left( \varrho; \frac{\beta_1 \mu_1 - \beta \mu}{\beta_1 - \beta}, \frac{\beta_1 B_1 - \beta B}{\beta_1 - \beta} \right)$$

*and consequently $H(\varrho; \mu, B) < +\infty$.*

[3] The locally uniform topology is defined by the set of neighbourhoods

$$\mathscr{V}(\varrho; \Lambda, \varepsilon) = \left\{ \varrho' ; \sup_{\substack{A \in \mathfrak{A}(\Lambda) \\ \|A\| = 1}} |\varrho(A) - \varrho'(A)| < \varepsilon \right\} \quad \text{for} \quad \Lambda \subset R^\nu, \ \varepsilon > 0 .$$

4. *The set $\Delta$ of all equilibrium states*

$$\Delta = \bigcup_{\substack{\beta > 0, \mu \\ B \in \mathscr{B}}} \Delta(\beta, \mu, B)$$

*is dense in the weak*-$\mathfrak{A}$ topology, in the set $E_G \cap \mathscr{V}$.*

*Proof*. Property 1 follows from the properties of $E_G \cap \mathscr{V}$ derived in Theorems 1 and 2 and the fact that $\varrho \in E_G \cap \mathscr{V}$ is affine and upper semi-continuous in the weak*-$\mathfrak{A}$ topology (cf. Theorem 4).

To deduce Property 3, we note that for each $\varrho \in E_G \cap \mathscr{V}$ we have

$$S(\varrho; \beta_1, \mu_1, B_1) = S(\varrho; \beta, \mu, B) + (\beta - \beta_1)\, H\left(\varrho; \frac{\beta_1 \mu_1 - \beta\mu}{\beta_1 - \beta}, \frac{\beta_1 B_1 - \beta B}{\beta_1 - \beta}\right).$$

Thus taking $\varrho \in \Delta(\beta, \mu, B)$ we find

$$S(\varrho; \beta_1, \mu_1, B_1) = P_S(\beta, \mu, B) + (\beta - \beta_1)\, H\left(\varrho; \frac{\beta_1 \mu_1 - \beta\mu}{\beta_1 - \beta}, \frac{\beta_1 B_1 - \beta B}{\beta_1 - \beta}\right)$$

and the desired inequality follows immediately. Taking $\beta_1 < \beta$, $\mu_1 = \mu$ and $B_1 = B$ we then find:

$$H(\varrho; \mu, B) \leqq (\beta - \beta_1)^{-1} [P_S(\beta_1, \mu, B) - P_S(\beta, \mu, B)]$$

and the boundedness of $H$ is an immediate consequence of the boundedness of $P_S$ (cf. Theorem 5 and Theorem 3 of I).

Next we note that this last estimate and the proof of Theorem 3 imply that if $\varrho \in \Delta(\beta, \mu, B)$ then for each parallelepiped $\Lambda_l$ there is a number $C_{\Lambda_l}(\beta, \mu, B)$ such that:

$$H_{\Lambda_l}(\varrho; \mu, B) \leqq C_{\Lambda_l}(\beta, \mu, B).$$

Property 2 is now a corollary of Theorems 3 and 6 of [17].

The proof of Property 4 is very similar to the proof given in [6] but care has to be taken about two points. First let us note that the argument of [16] can be repeated in the present context to show that for each $\mu$ $B \in \mathscr{B}$ the $G$-invariant hard core states with $H(\varrho; \mu, B) < +\infty$ are weak*-dense in $E_G \cap \mathscr{V}$. Thus it suffices to prove that each such state can be approximated by an equilibrium state. But if $\varrho \in E_G \cap \mathscr{V}$ and $H(\varrho; \mu, B)$ $< +\infty$ then the entropy $S(\varrho)$ of $\varrho$ defined by

$$S(\varrho) = S(\varrho; \beta, \mu, B) + \beta H(\varrho; \mu, B)$$

is such that $0 \leqq S(\varrho) < +\infty$. Hence we have

$$P_S(\beta, \beta^{-1}\mu, \beta^{-1}B) \geqq -\beta H(\varrho; \beta^{-1}\mu, \beta^{-1}B).$$

Thus the linear function $(\beta, \mu, B) \to -\beta H(\varrho; \beta^{-1}\mu, \beta^{-1}B)$ is such that its graph lies below the graph of the convex function

$$(\beta, \mu, B) \to P_S(\beta, \beta^{-1}\mu, \beta^{-1}B)$$

and the desired result appears to follow from Theorem 2 of [6]. However, this latter result depends upon a separability assumption which is not valid in the present case; $\mathscr{B}$ is not separable. Nevertheless we can choose $\mathscr{B}_1 \subset \mathscr{B}$ such that $\mathscr{B}_1$ is separable and each invariant hard core state is determined by its restriction to $\mathscr{B}_1$. Repeating the above definitions with $\mathscr{B}$ replaced by $\mathscr{B}_1$ we obtain a set $\Delta_1$ of equilibrium states and $\Delta_1 \subseteqq \Delta$. But now from [6] we deduce that $\Delta_1$, and consequently $\Delta$, is weak*-dense in $E_G \cap \mathscr{V}$.

We note that the arguments of [2] can also be applied to deduce that the set $T$ of $(\beta, \mu, B)$ such that the graph of $P_S$ has a unique tangent plane, and consequently such that $\Delta(\beta, \mu, B)$ reduces to one state $\varrho_{\beta,\mu,B}$ is a residual set in $R_+ \times R \times \mathscr{B}_1$. Thus the one significant result of [4, 6] which we have not obtained is the deduction that for $(\beta, \mu, B) \in T$ the unique equilibrium state $\varrho_{\beta,\mu,B}$ is given as an infinite volume limit of an appropriate state of the finite system. This last result would follow, however, from Theorem 5 if we could establish that $P = P_S$, or $P_\infty = P_S$, or $P = P_\infty$. This last form of equality is the one crucial remaining result necessary to the completion of the discussion of equilibrium states.

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S. Miracle-Sole and D. W. Robinson
Centre de Physique Théorique, C.N.R.S.
31, Chemin J. Aiguier
F-13 Marseille (9°)