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MEAN ENTROPY OF STATES IN QUANTUM STATISTICAL MECHANICS

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A B S T R A C T

The equilibrium states for an infinite system of quantum mechanics may be represented by states over suitably chosen C^* algebras. We consider the problem of associating an entropy with these states and finding its properties, positivity, sub-additivity, etc. For the states of a quantum spin system a mean entropy is defined and it is demonstrated that this entropy has certain properties of affinity, upper semi-continuity, etc.

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0. INTRODUCTION

In the algebraic theory of statistical mechanics the class of possible equilibrium states is defined as the subclass K of states ρ, over the C^* algebra $\mathfrak{A}$ of local observables, which satisfy certain subsidiary conditions of a physical origin. Firstly it is assumed that the theory is invariant under a symmetry group G (the translation group R^ν, for example) then the states $\rho \in K$ considered are taken to be G invariant. Secondly, as one wishes to describe only systems with a finite number of particles in each finite subsystem, extra conditions must be introduced. The consequence of these latter "finite mean density" conditions can be described as follows. If $\Lambda \subset R^\nu$ is an open set of compact closure and $\mathfrak{A}(\Lambda) \subset \mathfrak{A}$ the corresponding subalgebra of strictly local observables then a state $\rho \in K$ must be such that its restriction to each $\mathfrak{A}(\Lambda)$ is described by a density matrix ρ_Λ acting on a Hilbert space $\mathcal{H}_\Lambda$. As a direct result of this last property we may introduce, for each $\rho \in K$, a family of entropies $S(\rho_\Lambda)$ by the definition $S(\rho_\Lambda) = -\mathrm{Tr}_{\mathcal{H}_\Lambda}(\rho_\Lambda \log \rho_\Lambda)$. Consequently we may study properties of $S(\rho_\Lambda)$, attempt to introduce for each $\rho \in K$ an entropy per unit volume $\bar{S}(\rho)$, and, subsequently, analyse the linearity and continuity properties etc., of $\bar{S}(\rho)$.

The programme outlined above was recently completed by Ruelle, in collaboration with one of the present authors (D.W.R.), in the framework of classical statistical mechanics [1]. The purpose of the present paper is to attempt the same programme for quantum statistical mechanics. In this latter setting many difficulties arise due to non-commutativity and our results are complete only in the case of quantum spin systems. In the general case many interesting problems remain open.

1. GENERAL FORMULATION

We want to investigate both continuous infinite quantum statistical systems and lattice systems. Thus, we consider a C^* algebra $\mathfrak{A}$ and a collection $\{ \mathfrak{A}(\Lambda) \}$ of C^* sub-algebras of $\mathfrak{A}$, where Λ runs over

i) the bounded open sets in R^ν for continuous systems;

ii) the finite subsets of Z^ν for lattice systems.

We suppose that these sub-algebras satisfy the following axioms:

0) $\mathfrak{A}(\Lambda_1) \subset \mathfrak{A}(\Lambda_2)$ if $\Lambda_1 \subset \Lambda_2$.

1) For each Λ, $\mathfrak{A}(\Lambda)$ is isomorphic to $\mathcal{L}(\mathcal{H}_\Lambda)$ for some Hilbert space $\mathcal{H}_\Lambda$. We will usually identify $\mathfrak{A}(\Lambda)$ with $\mathcal{L}(\mathcal{H}_\Lambda)$ although this is not strictly compatible with 0).

2) $\mathfrak{A}$ is the norm closure of $\bigcup_\Lambda \mathfrak{A}(\Lambda)$.

3) $\mathfrak{A}(\Lambda_1 \cup \Lambda_2)$ is generated by $\mathfrak{A}(\Lambda_1) \cup \mathfrak{A}(\Lambda_2)$ in the weak operator topology on $\mathcal{L}(\mathcal{H}_{\Lambda_1 \cup \Lambda_2})$.

4) Let G denote the group of translations, i.e., $G = Z^\nu$ for lattice systems and $G = R^\nu$ for continuous systems. Then G acts on $\mathfrak{A}$ by automorphisms τ_x in such a way that $\tau_x(\mathfrak{A}(\Lambda)) = \mathfrak{A}(\Lambda + x)$, for all regions Λ and translations x.

Finally, we need a condition expressing the independence of observables belonging to disjoint regions. This condition may take one of two forms, depending on whether we are considering bosons or fermions:

5) Either

a. If Λ_1 and Λ_2 are any two disjoint regions, then $\mathfrak{A}(\Lambda_1)$ commutes with $\mathfrak{A}(\Lambda_2)$

or

b. Each $\mathfrak{A}(\Lambda)$ is generated by a set of creation and annihilation operators satisfying the canonical anticommutation relations, and, if Λ_1 and Λ_2 are disjoint regions, the creation and annihilation operators for Λ_1 anticommute with those for Λ_2.

These axioms describe several kinds of physical systems:

1) Ordinary continuous quantum systems, either bosons or fermions.

2) Quantum lattice systems, again either bosons or fermions, with finitely many creation and annihilation operators associated with each lattice site. For fermion lattice systems, $\mathcal{H}_\Lambda$ is finite dimensional for each finite set Λ, but for boson systems this is, of course, not true.

3) Quantum spin systems. In this case, $\mathcal{H}_\Lambda$ is finite dimensional for each bounded region Λ, but the different unit rays in $\mathcal{H}_{\{x\}}$, where x is a lattice point, are interpreted as describing different polarization states of a particle localized at x rather than varying occupation numbers for that point. We will assume that such systems satisfy axiom 5)a.

The statistical mechanical states of $\mathfrak{A}$ are those which, when restricted to an $\mathfrak{A}(\Lambda)$, are given by a density matrix. In other words, such a state ρ defines, for each region Λ, a positive operator ρ_Λ on $\mathcal{H}_\Lambda$, with $\mathrm{Tr}_{\mathcal{H}_\Lambda}(\rho_\Lambda) = 1$, such that

$$\rho(A) = \mathrm{Tr}_{\mathcal{H}_\Lambda}(\rho_\Lambda A)$$

if $A \in \mathfrak{A}(\Lambda) = \mathcal{L}(\mathcal{H}_\Lambda)$. This statement imposes no restriction on ρ if $\mathcal{H}_\Lambda$ is finite dimensional; otherwise, it corresponds to the requirement that there be only finitely many particles in each region Λ.

Every statistical mechanical state ρ defines a family $\{\rho_\Lambda\}$ of density matrices. Conversely, the assignment of a density matrix to each bounded region defines a statistical mechanical state on $\mathfrak{A}$, provided that the assignment satisfies the obvious compatibility condition that, if $\Lambda_1 \subset \Lambda_2$ and if $A \in \mathfrak{A}(\Lambda_1)$, then

$$\mathrm{Tr}_{\mathcal{H}_{\Lambda_1}}(\rho_{\Lambda_1} A) = \mathrm{Tr}_{\mathcal{H}_{\Lambda_2}}(\rho_{\Lambda_2} A)$$

We can reformulate the compatibility condition as follows: If $\Lambda_1 \subset \Lambda_2$, then $\mathfrak{A}(\Lambda_1)$ is a type I factor contained in $\mathfrak{A}(\Lambda_2) = \mathcal{L}(\mathcal{H}_{\Lambda_2})$. Hence, we may factorize

$$\mathcal{H}_{\Lambda_2} = \mathcal{H}_{\Lambda_1} \otimes \mathcal{H}'$$

in such a way that an operator A in $\mathfrak{A}(\Lambda_1) = \mathcal{L}(\mathcal{H}_{\Lambda_1})$ is identified with the operator $A \otimes 1$ on $\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}'$. [The space $\mathcal{H}'$ may be identified with $\mathcal{H}_{\Lambda_2 - \Lambda_1}$, but operators in $\mathfrak{A}(\Lambda_2 - \Lambda_1)$ do not factorize so nicely as those in $\mathfrak{A}(\Lambda_1)$ unless algebras for disjoint regions commute. See below.] The compatibility condition may now be formulated as:

$$\rho_{\Lambda_1} = \mathrm{Tr}_{\mathcal{H}'}(\rho_{\Lambda_2})$$

where $\mathrm{Tr}_{\mathcal{H}'}$ means the partial trace with respect to $\mathcal{H}'$, i.e., if $\{\varphi_i\}$ is an orthonormal basis for $\mathcal{H}_{\Lambda_1}$ and $\{\psi_i\}$ is an orthonormal basis for $\mathcal{H}'$, then

$$(\rho_{\Lambda_1}\varphi_i, \varphi_k) = \sum_{j=1}^{\infty} (\rho_{\Lambda_2}(\varphi_i \otimes \psi_j), \varphi_k \otimes \psi_j)$$

The condition that a state be translation invariant may easily be formulated in terms of the corresponding system of density matrices. For any region Λ and any translation x, τ_x is an isomorphism of $\mathfrak{A}(\Lambda)$ onto $\mathfrak{A}(\Lambda+x)$. Since $\mathfrak{A}(\Lambda)$ is identified with $\mathcal{L}(\mathcal{H}_\Lambda)$ and $\mathfrak{A}(\Lambda+x)$ with $\mathcal{L}(\mathcal{H}_{\Lambda+x})$, there is a unitary operator $U_{\Lambda,x}$ from $\mathcal{H}_\Lambda$ to $\mathcal{H}_{\Lambda+x}$ which induces this isomorphism, and $U_{\Lambda,x}$ is determined up to a multiplicative constant. Then the state defined by the system $\{\rho_\Lambda\}$ of density matrices is translation-invariant if and only if

$$\rho_{\Lambda+x} = U_{\Lambda,x}\,\rho_\Lambda\,U_{\Lambda,x}^{-1}$$

for all regions Λ and translations x.

We now want to make a more careful analysis of the relation of $\rho_{\Lambda_1 \cup \Lambda_2}$ to ρ_{Λ_1} and ρ_{Λ_2} when Λ_1 and Λ_2 are disjoint regions. We have already remarked that the inclusion of $\mathfrak{A}(\Lambda_1)$ in $\mathfrak{A}(\Lambda_1 \cup \Lambda_2)$ gives a factorization of $\mathcal{H}_{\Lambda_1 \cup \Lambda_2}$ as $\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}'$, where operators in $\mathfrak{A}(\Lambda_1)$ go over into operators of the form $A \otimes 1$. If we are considering a boson system or a spin system, then the commutant of $\mathfrak{A}(\Lambda_1)$ in $\mathfrak{A}(\Lambda_1 \cup \Lambda_2)$ is precisely $\mathfrak{A}(\Lambda_2)$. In this case, there is an essentially unique way to identify $\mathcal{H}'$ with $\mathcal{H}_{\Lambda_2}$, and operators in $\mathfrak{A}(\Lambda_2)$ take the form $1 \otimes A$ on $\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}_{\Lambda_2}$. Hence we have

$$\rho_{\Lambda_1} = \mathrm{Tr}_{\mathcal{H}_{\Lambda_2}}(\rho_{\Lambda_1 \cup \Lambda_2}) \quad , \quad \rho_{\Lambda_2} = \mathrm{Tr}_{\mathcal{H}_{\Lambda_1}}(\rho_{\Lambda_1 \cup \Lambda_2})$$

For fermion systems, although $\mathcal{H}'$ has the same dimension as $\mathcal{H}_{\Lambda_2}$, there is no unique sensible way to identify $\mathcal{H}'$ with $\mathcal{H}_{\Lambda_2}$. Nevertheless, by using the special structure of fermion systems, we can construct a useful identification of $\mathcal{H}'$ with $\mathcal{H}_{\Lambda_2}$. This we do as follows: Let N_1 and N_2 denote the number operators for the regions Λ_1 and Λ_2 respectively. Then a simple calculation with the anti-commutation relations shows that the commutant of $\mathfrak{A}(\Lambda_1)$ in $\mathfrak{A}(\Lambda_1 \cup \Lambda_2)$ is precisely $(-1)^{N_1 \cdot N_2}\, \mathfrak{A}(\Lambda_2)(-1)^{N_1 \cdot N_2}$. Therefore, we can identify $\mathcal{H}'$ with $\mathcal{H}_{\Lambda_2}$ in such a way that, if A is in $\mathfrak{A}(\Lambda_2) = \mathcal{L}(\mathcal{H}_{\Lambda_2})$, then A goes over into $(-1)^{N_1 \cdot N_2}(1 \otimes A)(-1)^{N_1 \cdot N_2}$, in $\mathcal{L}(\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}_{\Lambda_2})$. With this identification we have

$$\rho_{\Lambda_1} = \mathrm{Tr}_{\mathcal{H}_{\Lambda_2}}(\rho_{\Lambda_1 \cup \Lambda_2}) \qquad \rho_{\Lambda_2} = \mathrm{Tr}_{\mathcal{H}_{\Lambda_1}}\left((-1)^{N_1 \cdot N_2}\rho_{\Lambda_1 \cup \Lambda_2}(-1)^{N_1 \cdot N_2}\right)$$

The second of these equations can be simplified if we assume that ρ is an even state of $\mathfrak{A}$. By definition, an element A of some $\mathfrak{A}(\Lambda)$ is <u>odd</u> if

$$(-1)^{N(\Lambda)} A (-1)^{N(\Lambda)} = -A$$

where $N(\Lambda)$ is the number operator for the region Λ. A state ρ of $\mathfrak{A}$ is <u>even</u> if ρ vanishes on every odd element of every $\mathfrak{A}(\Lambda)$. If, now, ρ is an even state and A is an element of $\mathfrak{A}(\Lambda_2)$, then

$$\rho(A) = \mathrm{Tr}_{\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}_{\Lambda_2}} \left(\rho_{\Lambda_1 \cup \Lambda_2} (-1)^{N_1 \cdot N_2} (1 \otimes A) (-1)^{N_1 \cdot N_2} \right)$$

$$= \mathrm{Tr}_{\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}_{\Lambda_2}} \left(\rho_{\Lambda_1 \cup \Lambda_2} (1 \otimes A) \right)$$

To prove this equation, note that we can write A as the sum of an even part and an odd part, that the odd part contributes nothing to $\rho(A)$, and that the even part commutes with $(-1)^{N_1 \cdot N_2}$. Collecting these results we have:

<u>Proposition 1. Let ρ be a statistical-mechanical state of the C^* algebra $\mathfrak{A}$, and let $\{\rho_\Lambda\}$ be the corresponding system of density matrices. If $\mathfrak{A}$ is the algebra for a fermion system, we further assume that ρ is even. Then if Λ_1 and Λ_2 are disjoint regions, we may identify $\mathcal{H}_{\Lambda_1 \cup \Lambda_2}$ with $\mathcal{H}_{\Lambda_1} \otimes \mathcal{H}_{\Lambda_2}$ in such a way that</u>

$$\rho_{\Lambda_1} = \mathrm{Tr}_{\mathcal{H}_{\Lambda_2}}\left(\rho_{\Lambda_1 \cup \Lambda_2}\right) \qquad \rho_{\Lambda_2} = \mathrm{Tr}_{\mathcal{H}_{\Lambda_1}}\left(\rho_{\Lambda_1 \cup \Lambda_2}\right)$$

Note that, if we are dealing with a fermion system, then translation invariance implies that the state ρ is even. To show this *) let A be an odd element of some $\mathfrak{A}(\Lambda)$ and let x be a translation large enough so that $\Lambda + nx$ does not intersect Λ for $n = 1, 2, 3 \ldots$. Let

$$A_N = \frac{1}{N} \sum_{n=0}^{N-1} \tau_{nx} A$$

Now

$$\|A_N\|^2 = \|A_N^* A_N\| \leqslant \|\{A_N^*, A_N\}\| \leqslant \frac{1}{N^2} \sum_{n,m=0}^{N-1} \|\{(\tau_{nx}A)^*, \tau_{mx}A\}\|$$

$$\leqslant \frac{2}{N} \|A\|^2$$

where the last inequality is a consequence of

$$\{(\tau_{nx}A)^*, \tau_{mx}A\} = 0 \qquad \text{for } n \neq m$$

However due to translation invariance

$$\rho(A) = \rho(A_N) = \lim_{N \to \infty} \rho(A_N)$$

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*) This proof was independently discovered by R.T. Powers (unpublished).

But as $\lim_{N\to\infty} \frac{\|A\|}{N} = 0$ then $\lim_{N\to\infty} \rho(A_N) = 0$ and thus $\rho(A) = 0$.

Given a statistical-mechanical state ρ, and a region Λ, we can define the entropy of the region Λ as follows;

$$\begin{aligned} S(\rho_\Lambda) &= +\infty \quad \text{if } \rho_\Lambda \log \rho_\Lambda \text{ is not of trace class on } \mathcal{H}_\Lambda \\ &= -\mathrm{Tr}_{\mathcal{H}_\Lambda}(\rho_\Lambda \log \rho_\Lambda) \quad \text{otherwise.} \end{aligned}$$

In defining the operator $\rho_\Lambda \log \rho_\Lambda$ we use the usual convention $x \log x = 0$ for $x = 0$.

2. BASIC INEQUALITIES FOR THE ENTROPY

Lemma 1 *) Let A and B be positive, self-adjoint, trace class operators on a Hilbert space $\mathcal{H}$ then

$$\mathrm{Tr}_{\mathcal{H}}\left[A \log A - A \log B - A + B\right] \geqslant 0$$

Proof Let $\psi_i(\phi_i)$ be a complete orthonormal set of eigenfunctions of $A(B)$ and let $a_i(b_i)$ be the corresponding eigenvalues. Let $U = (u_{ij})$ be a unitary mapping defined by

$$\psi_i = \sum_{j=1}^{\infty} u_{ij} \phi_j$$

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*) This lemma, together with its proof, was communicated to one of us (D.W.R.) by Professor R. Jost who attributed it to O. Klein. If $\mathrm{Tr}(A) = \mathrm{Tr}(B) = 1$ this lemma is a particular case of theorem 1 of Ref. [2].

Now

$$(\psi_i | A \log A - A \log B | \psi_i) = a_i \left\{ \log a_i - \sum_{j=1}^{\infty} |u_{ij}|^2 \log b_j \right\}$$

$$\geqslant a_i \left\{ \log a_i - \log \sum_{j=1}^{\infty} |u_{ij}|^2 b_j \right\}$$

$$\geqslant a_i - \sum_{j=1}^{\infty} |u_{ij}|^2 b_j$$

$$= (\psi_i | A - B | \psi_i)$$

where to obtain the first inequality we have used the concavity of the logarithm and to obtain the second inequality we used

$$\log x \geqslant 1 - \frac{1}{x} \qquad (x > 0) .$$

The result follows by summation.

<u>Lemma 2</u> <u>Let A and B be positive, self-adjoint operators on a Hilbert space $\mathcal{H}$ then for $1 \geqslant \alpha \geqslant 0$</u>

$$(\alpha A + (1-\alpha)B) \log(\alpha A + (1-\alpha)B) \leqslant \alpha A \log A + (1-\alpha) B \log B$$

<u>and, further</u>

$$A \geqslant B \geqslant 0 \quad \text{implies} \quad \log A \geqslant \log B$$

The statements of the lemma are special consequences of the theory of convex and monotone operator functions initially developed by Löwner [3]. For further results the reader may consult Ref. [4]. The details of the application of the general theory to the case at hand are worked out in [5],[6]. Moreover we need the first inequality of the lemma, only with the operators replaced by their traces, and this can be proved without use of the general theory of convex operator functions [see [6],[7]].

We remark that Lemma 1 may be deduced from the first statement of Lemma 2. We preferred, however, to give the simple straightforward proof reproduced above.

The preceding lemmas may now be used to deduce the following results for the quantum entropy, specializations of which appear in [8],[9].

<u>Theorem 1. Let ρ be a statistical-mechanical state of the C^* algebra $\mathfrak{A}$, and let $\{\rho_\Lambda\}$ be the corresponding system of density matrices. If $\mathfrak{A}$ is the algebra for a fermion system we assume further that ρ is an even state. Then the associated entropy $S(\rho_\Lambda)$ is a positive set function, i.e.,</u>

$$S(\rho_\Lambda) \geqslant 0$$

<u>which is sub-additive, i.e.,</u>

$$S(\rho_{\Lambda_1 \cup \Lambda_2}) \leqslant S(\rho_{\Lambda_1}) + S(\rho_{\Lambda_2}) \quad , \Lambda_1 \cap \Lambda_2 = \phi .$$

<u>Further if $\{\rho_\Lambda^{(1)}\}$ and $\{\rho_\Lambda^{(2)}\}$ are two families of density matrices and $1 \geqslant \alpha \geqslant 0$ then</u>

$$\alpha S(\rho_\Lambda^{(1)}) + (1-\alpha) S(\rho_\Lambda^{(2)}) \leqslant S\left(\alpha\rho_\Lambda^{(1)} + (1-\alpha)\rho_\Lambda^{(2)}\right)$$

$$\leqslant \alpha S(\rho_\Lambda^{(1)}) + (1-\alpha) S(\rho_\Lambda^{(2)}) - \alpha\log\alpha - (1-\alpha)\log(1-\alpha)$$

<u>Proof</u> The positivity of $S(\rho_\Lambda)$ is an immediate consequence of the normalization of ρ_Λ and the fact that

$$-\lambda\log\lambda \geqslant 0 \qquad , \quad 1 \geqslant \lambda \geqslant 0 \quad .$$

The sub-additivity property follows from Lemma 1, Proposition 1 and the identification $\mathcal{H} = \mathcal{H}_{\Lambda_1} \otimes \mathcal{H}_{\Lambda_2}$, $A = \rho_{\Lambda_1 \cup \Lambda_2}$, $B = \rho_{\Lambda_1} \otimes \rho_{\Lambda_2}$. The final inequality is a consequence of Lemma 2. The lower bound is immediately obtained from the first statement of that lemma whilst the upper bound is obtained from the second statement as follows. We have

$$\alpha\rho_\Lambda^{(1)} + (1-\alpha)\rho_\Lambda^{(2)} \geqslant \alpha\rho_\Lambda^{(1)} \geqslant 0$$

and hence

$$\log\left(\alpha\rho_\Lambda^{(1)} + (1-\alpha)\rho_\Lambda^{(2)}\right) \geqslant \log\alpha\rho_\Lambda^{(1)}$$

Thus

$$-\alpha \operatorname{Tr}\left[\rho_\Lambda^{(1)} \log\left(\alpha\rho_\Lambda^{(1)} + (1-\alpha)\rho_\Lambda^{(2)}\right)\right] \leq -\alpha \operatorname{Tr}\left[\rho_\Lambda^{(1)} \log \alpha\rho_\Lambda^{(1)}\right]$$
$$= -\alpha \operatorname{Tr}\left[\rho_\Lambda^{(1)} \log \rho_\Lambda^{(1)}\right] - \alpha\log\alpha$$

and similarly

$$-(1-\alpha) \operatorname{Tr}\left[\rho_\Lambda^{(2)} \log\left(\alpha\rho_\Lambda^{(1)} + (1-\alpha)\rho_\Lambda^{(2)}\right)\right] \leq -(1-\alpha) \operatorname{Tr}\left[\rho_\Lambda^{(2)} \log (1-\alpha)\rho_\Lambda^{(2)}\right]$$
$$= -(1-\alpha) \operatorname{Tr}\left[\rho_\Lambda^{(2)} \log \rho_\Lambda^{(2)}\right] - (1-\alpha)\log(1-\alpha)$$

Adding the last two inequalities yields the desired result.

3. MEAN ENTROPY - THE QUANTUM LATTICE SYSTEM

The next desirable aim would be to define an entropy per unit volume, or mean entropy, by establishing, under suitable restrictions, the existence of $S(\rho_\Lambda)/V(\Lambda)$ in the limit of Λ increasing such that the volume $V(\Lambda) \to \infty$. Unfortunately we are at present able to do this solely for the case of a quantum lattice system and even then it is not possible to establish the existence of the limit in the most desirable generality. A possible means of improving our results is discussed in the concluding section.

Let us define for $a = (a_1, \ldots, a_\nu) \in Z^\nu$ and $a_1 > 0, \ldots, a_\nu > 0$ the parallelepiped $\Lambda(a)$ by

$$\Lambda(a) = \{ x \in Z^{\nu} ; \; 0 < x_i \leq a_i \text{ for } i = 1, 2, \ldots \nu \}$$

and the measure (volume) $V(\Lambda(a))$ of $\Lambda(a)$ is then given by $\prod_{i=1}^{\nu} a_i$.

<u>Theorem 2.</u> <u>If the family $\rho = \{\rho_\Lambda\}$ of density matrices of a quantum lattice system satisfies the conditions of normalization, compatibility, and translation invariance then the mean entropy</u>

$$S(\rho) = \lim_{a_1, \ldots a_\nu \to \infty} \frac{S(\rho_{\Lambda(a)})}{V(\Lambda(a))}$$

<u>exists, and in fact</u>

$$S(\rho) = \inf_{a_1, \ldots a_\nu} \frac{S(\rho_{\Lambda(a)})}{V(\Lambda(a))}$$

<u>Further, $S(\rho)$ is an affine function.</u> <u>Explicitly, if $\rho^{(1)} = \{\rho_\Lambda^{(1)}\}$ and $\rho^{(2)} = \{\rho_\Lambda^{(2)}\}$ are two appropriate families of density matrices and $1 \geqslant \alpha \geqslant 0$ then</u>

$$S\left(\alpha \rho^{(1)} + (1-\alpha)\rho^{(2)}\right) = \alpha \, S(\rho^{(1)}) + (1-\alpha) \, S(\rho^{(2)})$$

<u>Proof</u> Due to translation invariance $S(\Lambda(a))$ is a function of $a_1, \ldots, a_\nu$ only. Moreover, if we are dealing with a fermion system translation invariance implies that the state ρ is even (see Section 1). But if we introduce a function $S(a_1, \ldots, a_\nu)$ through the definition

$$S(a_1, \ldots, a_\nu) = S(\Lambda(a))$$

the sub-additivity of $S(\Lambda)$ implies that $S(a_1, \ldots, a_\nu)$ is sub-additive in each argument $a_i (1 \leq i \leq \nu)$ separately, i.e.,

$$S(a_1, \ldots, a_i^{(1)} + a_i^{(2)}, \ldots a_\nu) \leq S(a_1, \ldots, a_i^{(1)}, \ldots a_\nu) + S(a_1, \ldots, a_i^{(2)}, \ldots a_\nu)$$

A standard argument [cf., Lemma A1 [10]] establishes the existence of

$$S(\rho) = \lim_{a_1, \ldots a_\nu \to \infty} \frac{S(a_1, \ldots a_\nu)}{a_1 a_2 \ldots a_\nu} = \inf_{a_1, \ldots a_\nu} \frac{S(a_1, \ldots a_\nu)}{a_1 a_2 \ldots a_\nu}$$

The affine property of $S(\rho)$ follows from the last statement of Theorem 1 if one takes $\Lambda = \Lambda(a)$, divides by $V(\Lambda(a))$ and takes the appropriate limit.

4. PROPERTIES OF THE MEAN ENTROPY

For fermion lattice systems and spin systems we can exploit the finite dimensionality of the $\mathcal{H}_\Lambda$'s to prove some additional properties of the mean entropy.

Theorem 3. Let $\mathfrak{A}$ be the C^* algebra for a fermion lattice system or a spin lattice system. If x is a lattice point, let N denote the dimension of $\mathcal{H}_{\{x\}}$. Equip the set of states of $\mathfrak{A}$ with the weak * topology. Then

1) For any invariant state ρ of $\mathfrak{A}$, $0 \leq S(\rho) \leq \log N$.

2) The mean entropy is an upper semi-continuous function on the set of invariant states of $\mathfrak{A}$. If F is any closed subset of the set of invariant states of $\mathfrak{A}$, then the restriction of the mean entropy to F attains its maximum.

3) If ρ is an invariant state of $\mathfrak{A}$, and if μ_ρ is the unique probability measure with barycentre ρ concentrated on the extremal invariant states of $\mathfrak{A}$, then

$$S(\rho) = \int d\mu_\rho(\rho')\, S(\rho')$$

In physical language, statement 3 says that if ρ is an average of pure phases then the mean entropy of ρ is the same average of the entropies of the pure phases making up ρ. For the existence and uniqueness of the measure μ_ρ, see [11], Theorem 2, or [12], Theorem 3. We remark that, under the hypotheses of this theorem, $\mathfrak{A}$ is separable so there are no technical difficulties about the sense in which the measure is concentrated on the extremal invariant states.

<u>Proof</u> For any finite set Λ of lattice points, the dimension of $\mathcal{H}_\Lambda$ is $N^{V(\Lambda)}$. Now

$$S(\rho_\Lambda) = -\sum_{i=1}^{N^{V(\Lambda)}} \lambda_i \log \lambda_i$$

where the λ_i are the eigenvalues of ρ_Λ. By elementary estimates, if $\mu_1, \dots, \mu_n$ are positive real numbers with $\sum_i \mu_i = 1$, then

$$-\sum_{i=1}^{n} \mu_i \log \mu_i \leq \log n$$

Hence,

$$S(\rho_\Lambda) \leq \log N^{V(\Lambda)} = V(\Lambda) \log N$$

Dividing by $V(\Lambda)$ and taking the limit of infinite volume gives:

$$S(\rho) \leq \log N$$

Since $S(\rho)$ is non-negative by definition, we have proved 1).

To prove 2), observe first that the ρ_Λ's are continuous functions of ρ and that the eigenvalues of ρ_Λ vary continuously with ρ_Λ by perturbation theory. Since $-\lambda \log \lambda$ is a continuous function of λ,

$$S(\rho_\Lambda) = -\sum_i \lambda_i \log \lambda_i$$

is a continuous function of ρ . But

$$S(\rho) = \inf_{\Lambda} \left\{ \frac{S(\rho_\Lambda)}{V(\Lambda)} \right\}$$

where the infimum is to be taken over all rectangles. Thus, $S(\rho)$ is the infimum of a family of continuous functions and is therefore upper semi-continuous. In particular, if F is any closed set of invariant states on $\mathfrak{A}$, then the restriction of S to F takes on its maximum, since any upper semi-continuous function on a compact set takes on its maximum.

Furthermore, since $S(\rho)$ is both affine and upper semi-continuous, it respects barycentric decompositions. More precisely, if μ is any probability measure on the set of invariant states of $\mathfrak{A}$, and if the barycentre of μ is ρ , then

$$S(\rho) = \int d\mu(\rho') \, S(\rho') \quad .$$

(This follows from Lemma 10 of Ref. [13].) In particular, if μ_ρ is the unique decomposition of ρ into extremal invariant states *) then the above equation holds. This proves 3) and completes the proof of the theorem.

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*) Note that the uniqueness proofs given in Refs. [11),12)] for such decompositions are valid even for Fermi systems. In the Fermi case $\mathfrak{A}$ is R^ν (or Z^ν) Abelian, in the sense of [12)] as an argument similar to that appearing after Proposition 1 readily establishes.

5. CONCLUSION

Whilst in the case of a quantum spin system we have been able to obtain most of the desired results concerning the quantum entropy the position is less satisfactory in other cases. The main gap in the development is the failure to establish the existence of the mean entropy $S(\rho)$ under general circumstances. In classical statistical mechanics [1] these existence problems were solved by showing that the entropy satisfied a condition of strong sub-additivity. One could believe, and even support one's belief by heuristic physical arguments, that the same condition holds for the quantum entropy.

Conjecture. The quantum entropy $S(\rho_\Lambda)$ satisfies the inequality

$$S(\rho_{\Lambda_1 \cup \Lambda_2}) + S(\rho_{\Lambda_1 \cap \Lambda_2}) \leq S(\rho_{\Lambda_1}) + S(\rho_{\Lambda_2})$$

A satisfactory discussion of the existence of the mean entropy would ensue if this conjecture were proved. There would, however, still exist a problem in establishing a barycentric decomposition of the mean entropy in the general case because although it would clearly be an affine function it could not be expected to be an upper semi-continuous function.

We have not discussed in any detail the physical relevance of the mean entropy which we have introduced but postpone this to a forthcoming publication [14].

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