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Equivalence of ensembles in quantum lattice systems

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ABSTRACT. — A thermodynamic limit of a quantum lattice system is considered in the microcanonical, the canonical and the grand canonical ensembles. It is shown that we can deduce some properties in one ensemble if they are proved in another.

It is shown that the van Hove limit of the thermodynamic functions exists in the canonical and microcanonical formalism and also a property of convexity and monotony in the microcanonical ensemble.

1. INTRODUCTION

To describe macroscopic phenomena in equilibrium statistical mechanics, one can consider several ensembles namely the microcanonical, the canonical and the grand canonical ensemble. They differ essentially by the choice of basic macroscopic variables.

It is interesting to show the equivalence of their formalisms, i. e. that they describe macroscopic phenomena in equivalent manners. Actually this allows us to show some properties in one ensemble if they are proved in another. This article gives some such examples in the case of quantum lattice systems.

We consider a quantum lattice system on Z^ν. We associate with each lattice site $x \in Z^\nu$ a Hilbert space $\mathscr{H}_x$ of dimension two, and with each finite region Λ in Z^ν the tensor product

$$\mathscr{H}(\Lambda) = \bigotimes_{x \in \Lambda} \mathscr{H}_x$$

If $\Lambda_1 \subset \Lambda_2$ we can identify each bounded operator A on $\mathscr{H}(\Lambda_1)$ with $A \otimes 1_{\Lambda_2/\Lambda_1}$ on $\mathscr{H}(\Lambda_2)$, where $1_{\Lambda_2/\Lambda_1}$ is the identity of $\mathscr{H}(\Lambda_2/\Lambda_1)$. With this convention one defines the algebra of observables by the following

$$\mathscr{A} = \overline{\bigcup_{\Lambda \in Z^\nu} \mathscr{A}(\Lambda)}^{\|\ \|}$$

when $\mathscr{A}(\Lambda)$ is the set of bounded operators on $\mathscr{H}(\Lambda)$.

We note that the group Z^ν of space translations is a subgroup of the automorphism group of $\mathscr{A}$ and we denote the action of this group by $A \in \mathscr{A}(\Lambda) \to \tau_a A \in \mathscr{A}(\Lambda + a)$, $a \in Z^\nu$.

We consider interactions, i. e. functions Φ from the set of finite subsets of Z^ν to $\mathscr{A}$ such that

i) $\Phi(X) \in \mathscr{A}(X), \quad \forall X \subset Z^\nu$

ii) $\Phi(X)$ is hermitian

iii) $\Phi(X + a) = \tau_a \Phi(X), \quad \forall a \in Z^\nu$

iv) $$\|\Phi\| = \sum_{X \ni 0} \frac{\|\Phi(X)\|}{N(X)} < +\infty$$

where the last sum extends over all finite subsets of Z^ν containing 0 and N(X) is the number of points of X.

We denote by $\mathscr{B}$ the set of such interactions and $\mathscr{B}_0$ the set of finite range interactions, i. e. the dense subset of $\mathscr{B}$ containing those Φ for which there exists a finite $\Lambda_\Phi \subset Z^\nu$ such that $\Phi(X \cup \{0\}) = 0$ unless $X \subset \Lambda_\Phi$.

We note $\Phi \leqslant \Psi$, $\Phi, \Psi \in \mathscr{B}$ if $\Phi(X) \leqslant \Psi(X)$ for all $X \subset Z^\nu$.

We consider a system of particles on the finite set Λ and the energy operator $U_\Phi(\Lambda) \in \mathscr{A}(\Lambda)$ corresponding to the interaction Φ, defined by

$$U_\Phi(\Lambda) = \sum_{X \subset \Lambda} \Phi(X)$$

Further we denote by $\{e_0^{(x)}, e_1^{(x)}\}$ an orthonormal basis of $\mathscr{H}_x$, for each $x \in Z^\nu$.

Now, for each finite region $\Lambda \subset Z^\nu$, we define a configuration $|X\rangle$

which is at once a subset $\{ x_1, \ldots, x_k \}$ of Λ and an element of $\mathscr{H}(\Lambda)$ defined by

$$| X \rangle = \bigotimes_{x \in \Lambda} e^{(x)}_{\delta(x)}$$

where $\delta(x) = 1$ if $x \in \{ x_1, \ldots, x_k \}$ and 0 if not.

If $\Lambda_1 \subset \Lambda_2$ we can identify every configuration $| X \rangle$ of $\mathscr{H}(\Lambda_1)$ with $| X \rangle \otimes \phi_{\Lambda_2/\Lambda_1}$ of $\mathscr{H}(\Lambda_2)$, where $\phi_{\Lambda_2/\Lambda_1}$ is the vacuous subset of Λ_2/Λ_1. Clearly the set of all configurations of Λ is an orthonormal basis of $\mathscr{H}(\Lambda)$.

We define projectors $P^N(\Lambda) \in \mathscr{A}(\Lambda)$, $0 \leqslant N \leqslant N(\Lambda)$, by

$$\begin{aligned} P^N(\Lambda) | X \rangle &= | X \rangle \quad \text{if} \quad N(X) = N \\ &= 0 \quad \text{if} \quad \text{not} \end{aligned}$$

We consider interactions ϕ such that

$$\forall X \subset \mathbb{Z}^\nu, \ [\phi(X), \ P^N(X)]_- = 0, \qquad N = 0, 1, \ldots, N(X).$$

In order to consider thermodynamic limits we denote by $\{ \Lambda_m \}$, $m = 0, 1, 2, \ldots$ the sequences of cubes of Z with volume given by $(2^m L_0)^\nu$. L_0 being any integer and being constructed in such a manner that Λ_m contains Z^ν disjoints copies of Λ_{m-1}. Next we shall consider the limit of Λ going to infinity in the sense of van Hove (*).

2. ENSEMBLES

First we give a review of definitions and some results in the three ensembles which will be used in the following.

2.1. The microcanonical ensemble.

In the microcanonical formalism variables are the energy per unit of volume e, and the density n, $0 \leqslant n \leqslant 1$.

For each finite region Λ of Z^ν and interaction $\Phi \in \mathscr{B}$, we can define the microcanonical partition function by

$$\Omega^\Phi_\Lambda(E, N) = \operatorname{Tr}_{\mathscr{H}(\Lambda)} \left\{ P^N(\Lambda) \sum_{\lambda_i(\Phi,\Lambda) \leqslant E} E_{\lambda_i(\Phi,\Lambda)} \right\}$$

where $E = e.N(\Lambda)$, N is an integer such that $0 \leqslant N \leqslant N(\Lambda)$ and $\{ \lambda_i(\Phi, \Lambda) \}_{i \geqslant 0}$ is the set of eigenvalues of $U_\Phi(\Lambda)$ repeated according to multiplicity and $\{ E_{\lambda_i(\Phi,\Lambda)} \}_{i \geqslant 0}$ is the corresponding set of spectral projectors.

(*) See, for example [4], p. 13.

We define the microcanonical thermodynamic function, actually the entropy, by

$$s_\Lambda^\Phi\left(e, \frac{N}{N(\Lambda)}\right) = \frac{1}{N(\Lambda)} \log \Omega_\Lambda^\Phi(e.N(\Lambda), N)$$

For each $\Lambda \subset Z^\nu$ and $\Phi \in \mathscr{B}$ this is an increasing function of e and we can define an « inverse » function [1],

$$e_\Lambda^\Phi\left(S, \frac{N}{N(\Lambda)}\right)$$

We can extend (*) this function by linearity with respect to the second variable, to all n such that $0 \leqslant n \leqslant 1$.

Furthermore we know that the following is true.

THEOREM 1. — *Let $\Phi \in \mathscr{B}$. The following limits exist and are finite*

$$e^\Phi(s, n) = \lim_{m\to\infty} e_{\Lambda_m}^\Phi(s, n)$$
$$s^\Phi(e, n) = \lim_{m\to\infty} s_{\Lambda_m}^\Phi(e, n)$$

Furthermore, if Φ, $\Psi \in \mathscr{B}$

$$| e^\Phi(s, n) - e^\Psi(s, n) | \leqslant || \Phi - \Psi ||$$

The first statement is proved by combining the arguments of [1] and [2]. The last inequality follows from the following

$$| \mu_i[A] - \mu_i[B] | \leqslant || A - B ||$$

where A and B are $n \times n$ matrices and $\{ \mu_i[A] \}_{i \geqslant 0}$ (resp. $\{ \mu_i[B] \}_{i \geqslant 0}$ is the set of eigenvalues of A (resp. B) in increasing order and repeated according to multiplicity.

2.2. **The canonical ensemble.**

In the canonical formalism variables are the density n and the inverse temperature β.

For each finite region $\Lambda \subset Z^\nu$ and interaction $\Phi \in \mathscr{B}$, we can also define a canonical partition function

$$\Xi_\Lambda^\Phi(N, \beta) = \mathrm{Tr}_{\mathscr{H}(\Lambda)} \{ P^N(\Lambda) \exp(-\beta U_\Phi(\Lambda)) \}$$

where N is an integer such that $0 \leqslant N \leqslant N(\Lambda)$.

(*) As in [2] for the canonical case.

We define the canonical thermodynamic function, actually the free energy, by

$$f_{\Lambda}^{\Phi}\left(\frac{N}{N(\Lambda)}, \beta\right) = -\beta^{-1}\frac{1}{N(\Lambda)}\log \Xi_{\Lambda}^{\Phi}(N, \beta)$$

and as in the microcanonical case one can extend this function by linearity with respect to the first variable, to all n such that $0 \leqslant n \leqslant 1$. Furthermore we know that the following is true.

THEOREM 2. — *Let $\Phi \in \mathscr{B}$. The following limit exists and is finite*

$$f^{\Phi}(n, \beta) = \lim_{m\to\infty} f_{\Lambda_m}^{\Phi}(n, \beta)$$

Furthermore the fonction $\Phi \to f^{\Phi}(n, \beta)$ is concave and decreasing, and for $\Phi, \Psi \in \mathscr{B}$

$$|f^{\Phi}(n, \beta) - f^{\Psi}(n, \beta)| \leqslant ||\Phi - \Psi||$$

The first statement is proved as in [*2*]. The proofs of the remaining statements are identical to those of [*3*].

2.3. **The grand canonical ensemble.**

In the grand canonical formalism variables are the inverse temperature β and the chemical potential μ.

For each finite region $\Lambda \subset Z^{\nu}$ and interaction $\Phi \in \mathscr{B}$, we can also define a grandcanonical partition function

$$Z_{\Lambda}^{\Phi}(\beta, \mu) = \mathrm{Tr}_{\mathscr{H}(\Lambda)}\{\exp(\beta\mu\eta(\Lambda) - \beta U_{\Phi}(\Lambda))\}$$

where $\eta(\Lambda) \in \mathscr{A}(\Lambda)$ is defined by

$$\forall X \subset \Lambda \qquad \eta(\Lambda)|X\rangle = N(X)|X\rangle$$

We define the grandcanonical thermodynamic function, actually the pressure, by

$$p_{\Lambda}^{\Phi}(\beta, \mu) = \beta^{-1}\frac{1}{N(\Lambda)}\log Z_{\Lambda}^{\Phi}(\beta, \mu)$$

Then we know that the following is true.

THEOREM 3. — *Let $\Phi \in \mathscr{B}$. The following limit exists and is finite*

$$p_{\Lambda}^{\Phi}(\beta, \mu) = \lim_{\Lambda\to\infty} p_{\Lambda}^{\Phi}(\beta, \mu)$$

where $\Lambda \to \infty$ in the sense of van Hove.

Furthermore the function $\Phi \to p^{\Phi}(\beta, \mu)$ *is convex and increasing and for* $\Phi, \Psi \in \mathscr{B}$

$$| p^{\Phi}(\beta, \mu) - p^{\Psi}(\beta, \mu) | \leqslant || \Phi - \Psi ||$$

See [3] for the proof of this theorem.

2.4. Equivalence of ensembles.

We shall consider the following connection between the above formalisms:

THEOREM 4. — *Let* $\Phi \in \mathscr{B}$. *Therefore*

$$f^{\Phi}(n, \beta) = \sup_{\mu \in \mathbf{R}} \{ \mu n - p^{\Phi}(\beta, \mu) \}$$

In the quantum lattice system case we can prove, using only the previous definitions the following statement

$$p^{\Phi}(\beta, \mu) = \sup_{0 \leqslant n \leqslant 1} \{ \mu n - f^{\Phi}(n, \beta) \} \tag{4.1}$$

In particular, it is easy to prove that

$$\forall n, \qquad 0 \leqslant n \leqslant 1, \qquad \Lambda \subset \mathbf{Z}^{\nu}$$

$$p_{\Lambda}^{\Phi}(\beta, \mu) \geqslant \mu n - f_{\Lambda}^{\Phi}(n, \beta) \tag{4.2}$$

From (4.2) and Theorems 2 and 3, we find immediately

$$f^{\Phi}(n, \beta) \geqslant \sup_{\mu \in \mathbf{R}} \{ \mu n - p^{\Phi}(\beta, \mu) \} \tag{4.3}$$

Now $f^{\Phi}(., \beta)$ is a convex function of n, so for β and Φ fixed

$$\forall n \in [0, 1] \quad \exists \mu_n \in \mathbf{R} \quad \forall l \in [0, 1] \quad f^{\Phi}(l, \beta) \geqslant f^{\Phi}(n, \beta) - \mu_n(n - l) \tag{4.4}$$

Therefore, for each n

$$\begin{aligned} \sup_{\mu \in \mathbf{R}} \{ \mu n - p^{\Phi}(\beta, \mu) \} &\geqslant \mu_n n - p^{\Phi}(\beta, \mu_n) \\ &= \mu_n n - \sup_{0 \leqslant n \leqslant 1} \{ \mu_n n - f^{\Phi}(n, \beta) \} \\ &= \mu_n n - \mu_n l + f^{\Phi}(l, \beta) \\ &\geqslant f^{\Phi}(n, \beta) \end{aligned} \tag{4.5}$$

where we have used (4.1) and (4.4) and, in the second step, the fact that we take a supremum of a continuous function on a compact. Combining (4.3) and (4.5), the Theorem yields.

Remark. — We have also proved that for each n, there exists at least one $\mu_n \in \mathrm{R}$, actually the angular coefficient of a tangent line in n, such that

$$f^{\Phi}(n, \beta) = \mu_n n - p^{\Phi}(\beta, \mu_n) \tag{4.6}$$

Assuming differentiability of $f^{\Phi}(., \beta)$ at n, i. e. no phase transition, yields the standard thermodynamic relation

$$\mu = \frac{\partial f^{\Phi}(n, \beta)}{\partial n} \tag{4.7}$$

For sake of simplicity the case of derivative $-\infty$ at $n = 0$ and $+\infty$ at $n = 1$ was excluded, but it is easy to derive, in this case, the same result for $n = 1$ and we can take this formulas as definitions for $n = 0$. It is easy to find a similar result in the opposite direction, starting with (4.1).

THEOREM 5. — *Let $\Phi \in \mathscr{B}$. Therefore*

$$e^{\Phi}(s, n) = \sup_{\beta > 0} \{ f^{\Phi}(n, \beta) + s\beta^{-1} \}$$

The proof is identical to the previous one.

3. OTHER PROPERTIES

Now we shall consider some properties which follow from the previous sections.

PROPOSITION 1. — *Let $\Phi \in \mathscr{B}$, $\beta > 0$ and n such that $0 \leqslant n \leqslant 1$. Then the following limit exists and is finite:*

$$\lim_{\Lambda \to \infty} f_{\Lambda}^{\Phi}(n, \beta)$$

where $\Lambda \to \infty$ in the sense of van Hove.

First we prove the proposition for $\Phi \in \mathscr{B}_0$. Let Λ a finite region in the lattice, $\Lambda_m^{(i)}$, $i = 1, 2, \ldots, \mathrm{N}_m^-(\Lambda)$ the translated of Λ_m contained in Λ and $\Gamma_m = \bigcup_i \Lambda_m^{(i)}$; using subadditivity of $f_{\Lambda}^{\Phi}(n, \beta)$, we have

$$\begin{aligned} \mathrm{N}(\Lambda) f_{\Lambda}^{\Phi}(n, \beta) - \mathrm{N}_m^-(\Lambda) . \mathrm{N}(\Lambda_m) f_{\Lambda_m}^{\Phi}(n, \beta) \\ \leqslant \mathrm{N}(\Lambda/\Gamma_m) f_{\Lambda/\Gamma_m}(n, \beta) + \Delta \| \phi \| [\mathrm{N}_m^-(\Lambda)\mathrm{S}_m + \mathrm{N}(\Lambda/\Gamma_m)] \end{aligned}$$

where $\mathrm{S}_m = 2\nu(2^m\mathrm{L}_0)^{\nu-1}$ and Δ is the range of Φ, i. e. the diameter of Λ_{Φ}.

Therefore $\forall \varepsilon > 0\ \exists M\ \forall m \geqslant M$ and Λ large enough in the sense of van Hove

$$f_\Lambda^\Phi(n, \beta) \leqslant f_{\Lambda_m}^\Phi(n, \beta) + \varepsilon \leqslant f^\Phi(n, \beta) + 2\varepsilon$$

Furthermore $\forall \Lambda$

$$\mu n - p_\Lambda^\Phi(\beta, \mu) \leqslant f_\Lambda^\Phi(n, \beta)$$

But $p_\Lambda^\Phi(\beta, \mu)$ tends to $p^\Phi(\beta, \mu)$ when $\Lambda \to \infty$ in the sense of van Hove, hence $\forall \varepsilon > 0$ and Λ large enough in the sense of van Hove,

$$\mu n - p^\Phi(\beta, \mu) - \varepsilon \leqslant f_\Lambda^\Phi(n, \beta), \qquad \forall \mu$$

Moreover

$$f^\Phi(n, \beta) - \varepsilon = \sup_{\mu \in \mathbb{R}} \{ \mu n - p^\Phi(\beta, \mu) \} - \varepsilon \leqslant f_\Lambda^\Phi(n, \beta)$$

We extend the property to $\Phi \in \mathscr{B}$ using the equicontinuity of f_Λ^Φ in Φ.

PROPOSITION 2. — *Let $\Phi \in \mathscr{B}$, n such that $0 \leqslant n \leqslant 1$. The following limit exists and is finite*

$$e^\Phi(s, n) = \lim_{\Lambda \to \infty} e_\Lambda^\Phi(s, n)$$

when Λ tends to infinity in the sense of van Hove. Furthermore the function $\Phi \to e^\Phi(s, n)$ is concave and decreasing.

We prove the existence of the limit as previously. Concavity follows from the concavity of $f^\Phi(n, \beta)$. Hence, if $\Phi, \Psi \in \mathscr{B}$ and $0 \leqslant \lambda \leqslant 1$

$$\begin{aligned} \lambda e^\Phi(s, n) + (1 - \lambda) e^\Psi(s, n) &\geqslant \sup_{\beta > 0} \{ \lambda f^\Phi(n, \beta) + (1 - \lambda) f^\Psi(n, \beta) + s\beta^{-1} \} \\ &\geqslant e^{\lambda\Phi + (1-\lambda)\Psi}(s, n) \end{aligned}$$

Moreover, if $\Phi \leqslant \Psi$

$$\begin{aligned} e^\Phi(s, n) &= \sup_{\beta > 0} \{ f^\Phi(n, \beta) + s\beta^{-1} \} \\ &\geqslant \sup_{\beta > 0} \{ f^\Psi(n, \beta) + s\beta^{-1} \} = e^\Psi(s, n) \end{aligned}$$

We can prove a similar proposition for the limit of $s_\Lambda^\Phi(e, n)$, which exists when Λ tends to infinity in the sense of van Hove and which is increasing and convex with respect to Φ.

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