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KMS Conditions and Local Thermodynamical Stability of Quantum Lattice Systems

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Abstract. We formulate local thermodynamical stability conditions for states of quantum lattice systems, and show that these conditions are implied by, and in the case of translationally invariant states equivalent to, those of Kubo-Martin-Schwinger (KMS).

1. Introduction

This paper is concerned with the relationship between certain local thermodynamic stability (LTS) conditions and the KMS conditions for quantum lattice systems.

The LTS conditions, which will be precisely specified below, may be described as follows. For each state ϕ of a system and each bounded region Λ , we define a conditional free energy $\tilde{F}_A(\phi)$ (cf. Definition 2.1): this quantity is a quantal generalisation of that defined in [1, 2] for classical systems, and is designed to represent the free energy of the "open system" consisting of the particles in Λ , interacting with one another and with the particles outside that region. We define the LTS conditions for ϕ (cf. Definition 2.2) to be that, for each bounded region Λ , $\tilde{F}_A(\phi)$ is minimal for variations in the state which leaves it unchanged outside Λ .

With these definitions, and under the assumption of tempered, translationally invariant, finite-body (or somewhat more general) interactions, we prove the following Theorem.

Theorem. (a) If a translationally invariant state satisfies the LTS conditions, it satisfies the KMS conditions.

(b) A state satisfying the LTS conditions is stationary in time.

(c) A state satisfies the LTS conditions if it satisfies the KMS conditions.

We shall adopt the notations of references [3, 4]. Thus, \mathfrak{A} denotes the C^{*}algebra of quasi-local observables of the system and $\mathfrak{A}(I)$ its subalgebra for the

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region I. We shall denote the set $\{\Lambda\}$ of bounded regions of the lattice by L. For $\Lambda \in L$, $N(\Lambda)$ denotes the number of points in Λ , Λ^c the region complementary to Λ . For a state ϕ of \mathfrak{A} , ϕ_I denotes its restriction to $\mathfrak{A}(I)$.

We define the energy observable \tilde{H}_{A} for $A \in L$ by the formula

$$\tilde{H}_{A} = U(A) + W_{A}, \tag{1.1}$$

where $U(\Lambda)$, W_A are as specified in [3]: they respectively represent the interaction energy between the particles in Λ , and the energy of interaction between the particles in Λ and those in Λ^c . The time translation automorphism of \mathfrak{A} is denoted by σ_i . For $A \in \mathfrak{A}(\Lambda)$,

$$(d/dt)\sigma_t(A)_{|t=0} = i[\tilde{H}_A, A].$$

$$(1.2)$$

The assumptions on the interaction potential relevant to all our results (apart from the trivial convention that the interaction potential for trivial region is zero) are as follows. In order to be able to define W_A , we need a temperedness of the potential. It is also necessary that the time translation σ_t satisfying (1.2) exists. No other assumptions are needed for (c).

For (a), we use translational invariance of the potential in addition.

For (b), we use the assumption that the generator of σ_t is the closure of the (normal) derivation δ , defined on $\bigcup_{A \in L} \mathfrak{A}(A)$ by the formula

$$\delta(A) = i [\tilde{H}_A, A], \quad \forall A \in \mathfrak{U}(A).$$
(1.3)

These assumptions are satisfied, for example, in the case treated in [3] (see Theorem 4 in [5]).

All the arguments except (a) can be carried out in a more general setting, where σ_t is a continuous one-parameter group of automorphisms of a UHF algebra \mathfrak{A} (generated by an increasing sequence \mathfrak{A}_n of finite dimensional factors) such that the infinitesimal generator δ has a domain containing $\bigcup_n \mathfrak{A}_n$ and $\delta(A) = i [h_n, A] \forall A \in \mathfrak{A}_n$.

An essential tool in our discussion is the relative entropy introduced in [10] as follows. Let M be a von Neumann algebra and let $\hat{\psi}$ and $\hat{\phi}$ be normal positive linear functionals on M. We denote their support projections by $s(\hat{\psi})$ and $s(\hat{\phi})$, respectively. [In our application, we need the case where $\hat{\psi}$ is faithful, i.e. $s(\hat{\psi})=I$.] Let Ψ and Φ be representative vectors of $\hat{\psi}$ and $\hat{\phi}$ in a natural positive cone. Then the relative modular operator $\Delta_{\Phi,\Psi}$ is defined to be a positive selfadjoint operator with kernel $I - s^{M'}(\Psi)s^{M}(\Phi)$ satisfying the equation

$$\Delta_{\boldsymbol{\phi},\boldsymbol{\Psi}} = (S_{\boldsymbol{\phi},\boldsymbol{\Psi}} \mathbf{s}^{M'}(\boldsymbol{\Psi}))^* \, \bar{S}_{\boldsymbol{\phi},\boldsymbol{\Psi}} \mathbf{s}^{M'}(\boldsymbol{\Psi}) \,, \tag{1.4}$$

where $S_{\Phi,\Psi}$ is defined on $M\Psi$ by the equation

$$S_{\Phi \Psi} x \Psi = s^{M}(\Psi) x^{*} \Phi, \quad \forall x \in M$$

and where s^{M} and $s^{M'}$ denote the *M*-support and *M'* support, respectively, of a vector.

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The relative entropy $S(\hat{\psi}/\hat{\phi})$ is defined by

$$S(\hat{\psi}/\hat{\phi}) = \int_{+0}^{\infty} \log \lambda d(\Phi, E(\lambda)\Phi), \qquad (1.5)$$

$$\Delta_{\Phi \Psi} = \int \lambda dE(\lambda) \qquad (1.6)$$

if $s(\hat{\psi}) \ge s(\hat{\phi})$ [and hence $E(+0)\Phi = 0$]; and is defined to be $+\infty$ otherwise. When $\hat{\phi}$ and $\hat{\psi}$ are faithful, this definition coincides with that given in [4]. For positive linear functionals ψ and ϕ of the C*-algebra \mathfrak{A} , we define $S(\psi/\phi)$ to be given by $S(\hat{\psi}/\hat{\phi})$ if π_{ψ} quasi-contains π_{ϕ} , where $\hat{\psi}$ and $\hat{\phi}$ are the normal positive linear functionals of $\pi_{\psi}(\mathfrak{A})$ " satisfying $\hat{\psi}(\pi_{\psi}(A)) = \psi(A)$ and $\hat{\phi}(\pi_{\psi}(A)) = \phi(A)$ for all $A \in \mathfrak{A}$; and to be $+\infty$ otherwise.

The relative entropy $S(\psi/\phi)$ so defined is related to the conditional entropy \tilde{S}_A , defined below, by the following formula, proved in [10]:

$$\tilde{S}_{A}(\phi) = S(\omega'/\phi_{A^{c}}) - S(\tau_{A} \otimes \omega'/\phi)$$
(1.7)

where τ_A is the tracial state on $\mathfrak{A}(A)$ and where ω' is any state of $\mathfrak{A}(A^c)$ of which either $S(\omega'/\phi_A)$ or $S(\tau_A \otimes \omega'/\phi)$ is finite. In fact, if one of these relative entropies is finite, then so too is the other.

Properties of $S(\psi/\phi)$, which we shall use, are the following ones, proved in [10]:

If ψ and ϕ are two states, or positive continuous linear functionals with the same norm, then

$$S(\psi/\phi) \ge 0. \tag{1.8}$$

(The equality holds if and only if $\psi = \phi$.)

If ψ is a separating state on $\mathfrak{A}, h=h^*\in\mathfrak{A}$ and ψ^h denotes the perturbed state specified in [10], then

$$S(\psi^h/\phi) = -\phi(h) + S(\psi/\phi).$$
(1.9)

2. Relation of LTS to KMS

In a usual way we define the density matrix $\varrho_A^{\phi}(\in \mathfrak{A}(\Lambda))$ corresponding to the state ϕ on \mathfrak{A} and the region $\Lambda(\in L)$ by the formula

 $\phi(A) = \tau_A(\varrho_A^{\phi}A) \,\forall A \in \mathfrak{A}(A)$

and we define the entropy induced by ϕ on Λ to be

$$S_A(\phi) = -\tau_A(\varrho_A^\phi \log \varrho_A^\phi) \,. \tag{2.1}$$

Definition 2.1. The conditional entropy $\tilde{S}_A(\phi)$ and the conditional free energy $\tilde{F}_A^{\beta}(\phi)$, induced by the state ϕ on the region Λ , are defined by the following formulae:

$$\tilde{S}_{A}(\phi) = \lim_{A'\uparrow} \left[S_{A'}(\phi) - S_{A'\setminus A}(\phi) \right], \qquad (2.2)$$

$$\tilde{F}_{A}^{\ \beta}(\phi) = \phi(\tilde{H}_{A}) - \beta^{-1}\tilde{S}_{A}(\phi) \tag{2.3}$$

where β is a real positive constant, called the inverse temperature.

Definition 2.2. A state ϕ of \mathfrak{A} satisfies the LTS conditions if for each $\Lambda \in L$ and for every ψ satisfying $\psi_{\Lambda^c} = \phi_{\Lambda^c}$, the following inequality holds:

$$\tilde{F}_{A}^{\ \beta}(\phi) \leq \tilde{F}_{A}^{\ \beta}(\psi) \,. \tag{2.4}$$

Remark. Definitions 2.1 and 2.2 provide quantal generalisations of the definitions given in [1] for the conditional entropy, conditional free energy and local stability for classical lattice systems: for one can infer from the martingale theorem that Equation (7) and Definition 1 of [1] can be written in forms corresponding to the above Equations (2.3) and (2.4). Further, in the classical case, the local stability conditions correspond to the Dobrushin-Lanford-Ruelle equations.

Lemma 2.3. For any state ϕ of \mathfrak{A} , the following majorization holds:

$$\phi \leq d(\Lambda) \left(\tau_A \otimes \phi_{A_c} \right) \tag{2.5}$$

where $d(\Lambda)$ denotes the dimension of the algebra $\mathfrak{A}(\Lambda)$ (i.e. $d(\Lambda) = n^2$ if $\mathfrak{A}(\Lambda)$ is a type I_n factor).

Proof. Let $u_{ij}(i, j=1, ..., n)$ be a matrix unit for $A \in \mathfrak{A}(A)$. Then $A \in \mathfrak{A}$ can be written as $A = \sum u_{ij}A_{ij}, A_{ij} \in \mathfrak{A}(A^c)$.

Let

 $\phi_{ij}(x) \equiv \phi(u_{ij}x), \qquad x \in \mathfrak{A}(\Lambda^c).$

By the self-adjointness of ϕ , $\phi_{ii}(x)^* = \phi_{ii}(x^*)$. By the positivity of ϕ ,

 $\phi((u_{ki}x + cu_{kj}y)^* (u_{ki}x + cu_{kj}y)) \ge 0$

for $x, y \in \mathfrak{A}(\Lambda^c)$ and arbitrary complex number c. Thus

 $|\phi_{ij}(x^*y)|^2 \leq \phi_{ii}(x^*x)\phi_{jj}(y^*y)$.

Each ϕ_{ii} is positive and $\phi_{A^c} = \sum_i \phi_{ii}$.

Hence

$$\begin{split} \phi(A^*A) &= \sum_{i, j, k} \phi_{ij} (A^*_{ki} A_{kj}) \\ &\leq \sum_{i, j} \left\{ \sum_{k} (\phi_{ii} (A^*_{ki} A_{ki}))^{1/2} (\phi_{jj} (A^*_{kj} A_{kj}))^{1/2} \right\} \\ &\leq \sum_{i, j} \left(\sum_{k} \phi_{ii} (A^*_{ki} A_{ki}) \right)^{1/2} \left(\sum_{k} \phi_{jj} (A^*_{kj} A_{kj}) \right)^{1/2} \\ &\leq \left\{ \sum_{i} \phi_{ii} \left(\sum_{k} A^*_{ki} A_{ki} \right) \right\} \left\{ \sum_{i} 1 \right\} \\ &\leq n \phi_{A^c} \left(\sum_{i, k} A^*_{ki} A_{ki} \right) = n^2 (\tau_A \otimes \phi_{A^c}) (A^*A) \,. \end{split}$$
 QED.

Lemma 2.4. (1) The limit in (2.2) is always defined.

(2) For any state ϕ of \mathfrak{A} , $0 \ge \tilde{S}_A(\phi) \ge -\log d(A)$.

(3) \tilde{S}_A is a weakly upper semicontinuous concave function of ϕ .

(4) \tilde{F}_{A}^{β} is a weakly lower semicontinuous convex function of ϕ .

(5) For a given $\Lambda \in L$ and a state ω of $\mathfrak{A}(\Lambda^c)$, there exists a state ϕ of \mathfrak{A} such that $\phi_{\Lambda^c} = \omega$ and $\tilde{F}_{\Lambda}{}^{\beta}(\phi) \leq \tilde{F}_{\Lambda}{}^{\beta}(\psi)$ for all states of ψ satisfying $\psi_{\Lambda^c} = \omega$.

(6) $S_{\Lambda}(\phi) \ge \tilde{S}_{\Lambda}(\phi)$.

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Proof. (1) By the strong subadditivity of the entropy functional S_{Λ} (cf. [6]), $S_{\Lambda'}(\phi) - S_{\Lambda' \setminus \Lambda}(\phi)$ is monotone decreasing in Λ' as soon as Λ' contains Λ . Hence the limit is defined.

(2) Suppose $\Lambda' \supset \Lambda$. Then $\varrho_{\Lambda'\setminus\Lambda}^{\phi} = \varrho_{\Lambda'}^{\overline{\omega}}$ for $\overline{\omega} = \tau_{\Lambda} \otimes \phi_{\Lambda^c}$.

Hence by Klein's inequality (cf. [7])

$$S_{A'}(\phi) - S_{A'\setminus A}(\phi) = -\phi(\log \varrho_{A'}^{\phi} - \log \varrho_{A'}^{\bar{\omega}}) \leq 0.$$

$$(2.6)$$

By Lemma 2.3, $d(\Lambda)\bar{\omega} \ge \phi$, and hence $d(\Lambda)\bar{\omega}_{A'} \ge \phi_{A'}$, which is equivalent to $d(\Lambda)\varrho_{A'}^{\bar{\omega}} \ge \varrho_{A'}^{\phi}$.

By the operator monotone property of logarithm, we obtain

 $\log d(\Lambda) + \log \varrho_{\Lambda'}^{\overline{\omega}} \ge \log \varrho_{\Lambda'}^{\phi}$.

Hence

$$S_{A'}(\phi) - S_{A'\setminus A}(\phi) \ge -\log d(A) . \tag{2.7}$$

Estimates (2.6) and (2.7) establish (2).

(3) By the proof in (1), \tilde{S}_A is an infimum of weakly continuous function (2.6) and hence weakly upper semi-continuous. It is known [8] that

$$\tau_{A'}(\varrho_{A'}\log\varrho_{A'}-\varrho_{A'}\log\sigma_{A'}) \tag{2.8}$$

is convex jointly in $\sigma_{A'}$, $\varrho_{A'}$. Hence (2.6) is concave in ϕ , which implies the concavity of the limit.

(4) follows from (3).

(5) The existence follows from (4) and the compactness of the set of ψ 's satisfying $\psi_{A^c} = \omega$.

(6) follows from the subadditivity of entropy. QED.

Proof of Theorem. (a) Assume that ϕ is a translationally invariant state of \mathfrak{A} satisfying the LTS conditions. We apply Equation (2.4) to the case where $\psi = \omega^{G,A} \otimes \phi_{A^c}$, where

$$\omega^{G,\Lambda}(A) = \tau_{\Lambda}(Ae^{-\beta U(\Lambda)})/\tau_{\Lambda}(e^{-\beta U(\Lambda)}), \quad \forall A \in \mathfrak{A}(\Lambda).$$
(2.9)

Then it follows from the definition of \tilde{F}_A that

 $\tilde{F}_A(\psi) = -\beta^{-1} \log \tau_A(e^{-\beta U(A)}) + \psi(W_A).$

Hence Equations (2.3), (2.4) and Lemma 2.4 (6) imply that

 $S_{A}(\phi) - \beta \phi(U(A)) \ge \log \tau_{A}(e^{-\beta U(A)}) - 2 \|\beta W_{A}\|.$

On deviding this inequality by $N(\Lambda)$ and using the result in [3] that

 $\lim_{A'\uparrow} \|W_A\|/N(A) = 0,$

we obtain

$$\lim_{A\uparrow} N(A)^{-1} (S_A(\phi) - \beta \phi(U(A))) \ge \lim_{A\uparrow} N(A)^{-1} \log \tau_A(e^{-\beta U(A)}).$$

Since the opposite inequality holds for any ϕ , we obtain the equality which implies the KMS conditions for ϕ [9].

(b) Assume that ϕ satisfies the LTS conditions and apply (2.4) to the case where

 $\psi(\cdot) = \phi(e^{isA}(\cdot)e^{-isA})$

with
$$s \in R$$
 and $A = A^* \in \mathfrak{A}(\Lambda)$. Then it follows from (2.4) that

$$\phi(e^{isA}\tilde{H}_A e^{-isA}) \ge \phi(\tilde{H}_A)$$

for all $A = A^* \in \mathfrak{A}(\Lambda)$ and $\Lambda \in L$. Hence

$$\phi(i[H_A, A]) = 0$$

for all $A \in \mathfrak{A}(A)$. By (1.3),

 $\phi(\delta(A)) = 0 \tag{2.10}$

for all $A \in \mathfrak{A}(A)$ and for all $A \in L$. Hence it holds for all $A \in \mathfrak{A}$ in the domain of the infinitesimal generator δ of σ_t . For such A,

 $(d/dt) \sigma_t(A) = \delta(\sigma_t(A)).$

Equation (2.10) then proves that $\phi(\sigma_t(A))$ is independent of t for all A in the domain of δ , and hence for all $A \in \mathfrak{A}$.

(c) Let ψ be a state of \mathfrak{A} satisfying the KMS condition, and ω the restriction of ψ to $\mathfrak{A}(\Lambda^c)$.

Since the KMS conditions imply the Gibbs conditions, we have

$$\psi^{\beta H_A + cI} = \tau_A \otimes \phi' \tag{2.11}$$

where c is the normalization constant $(c = -\log \psi^{\beta \tilde{H}_A}(I))$ and ϕ' is some state of $\mathfrak{A}(\Lambda^c)$. By the formula (1.9),

$$S(\psi_2^h/\psi_1) = -\psi_1(h) + S(\psi_2|\psi_1)$$
(2.12)

and by the formula (1.7),

$$\tilde{S}_{A}(\psi_{1}) = -S(\tau_{A} \otimes \omega'/\psi_{1}) + S(\omega'/\omega)$$
(2.13)

for ψ_1 satisfying $(\psi_1)_{A_c} = \omega$, where (2.13) holds whenever either $S(\omega'/\omega)$ or $S(\tau_A \otimes \omega'/\psi_1)$ is finite (and then both are finite).

Hence

$$S(\psi/\psi_1) = S((\tau_A \otimes \phi')^{-(\beta \tilde{H}_A + cI)}/\psi_1)$$

= $c + \beta \psi_1(\tilde{H}_A) + S(\tau_A \otimes \phi'/\psi_1)$
= $c + \beta \psi_1(\tilde{H}_A) - \tilde{S}_A(\psi_1) + S(\phi'/\omega)$. (2.14)

For $\psi_1 = \psi$, we obtain

$$\beta \psi(\tilde{H}_{A}) - \tilde{S}_{A}(\psi) = -c - S(\phi'/\omega)$$

which proves that $S(\phi'/\omega)$ is finite. Substituting this into (2.14), we obtain

 $\beta(\tilde{F}_{\mathcal{A}}(\psi_1) - \tilde{F}_{\mathcal{A}}(\psi)) = S(\psi/\psi_1) \ge 0, \qquad (2.15)$

which proves the minimality of $\tilde{F}_{A}(\psi)$. QED.

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