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Stability for mean field models

by

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ABSTRACT. — For mean field models, we introduce the notion of stable KMS-states and prove the equivalence with relative minimum free energy state.

I. INTRODUCTION

For systems with short range interactions, much work has been done on the characterization of KMS-states by stability properties [1-6].

Much less has been done for long range interactions, because already the KMS-condition should be carefully stated in this case. We do not aim here this problem in its full generality, but restrict ourselves to the easier situation of mean field models on a lattice. In this situation we define the KMS-property via a correlation inequality which is meaningful (see [7]).

We extend to mean field systems the proof that global thermodynamic stability (or the variational problem) implies the KMS-property. We are also interested in the inverse implication. It is known from explicit examples (see e. g. [8-9]) that the inverse implication is not true. Therefore we introduce a supplementary condition, and KMS-state satisfying this condition are called stable KMS-states. We prove then that the stable KMS-property implies the relative thermodynamic stability property.

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II. STABILITY AND EQUILIBRIUM

Let \mathcal{H} be a Hilbert space, which we take finite dimensional for purely technical convenience; \mathcal{B} the set of bounded operators on \mathcal{H} , and \mathcal{B}^∞ the inductive limit C*-algebra of the finite C*-algebras $\mathcal{B}_\Lambda (\Lambda \subset \mathbb{Z}^v)$. For more details see [7].

Any density matrix ρ on \mathcal{H} defines a product state ω_ρ of \mathcal{B}^∞ by:

$$\omega_\rho(X_1 \otimes \dots \otimes X_n) = \prod_{i=1}^n \text{Tr } \rho X_i, \quad X_i \in \mathcal{B}.$$

Remark that the states ω_ρ are factor states and that if $\rho \neq \rho'$, the states ω_ρ and $\omega_{\rho'}$ are disjoint [10, 11].

Mean field models are defined by the local Hamiltonians H_Λ :

$$H_\Lambda = \sum_{i \in \Lambda} A_i + \frac{1}{2N(\Lambda)} \sum_{\substack{i \neq j \\ i, j \in \Lambda}} B_{ij} \quad (1)$$

where $A_i \in \mathcal{B}_{\{i\}}$ and all A_i ($i \in \Lambda$) are copies of $A = A^* \in \mathcal{B}$ and $B_{ij} \in \mathcal{B}_{\{ij\}}$ ($i, j \in \Lambda$) are copies of a self-adjoint B in $\mathcal{B} \otimes \mathcal{B}$ which is invariant under the permutation P on $\mathcal{H} \otimes \mathcal{H}$ defined by $P(\psi \otimes \phi) = \phi \otimes \psi$; $\psi, \phi \in \mathcal{H}$. As the local Hamiltonians are locally symmetric any limit Gibbs state will be a symmetric state. Therefore we restrict ourselves to this class S of states. For all $\omega \in S$ there exists a unique probability measure μ_ω on the set of density matrices on \mathcal{H} such that [12]:

$$\omega = \int d\mu_\omega(\rho) \omega_\rho \quad (2)$$

For any $\omega \in S$, the free energy density $f(\omega)$ is defined by

$$f_\beta(\omega) = e(\omega) - \beta^{-1}s(\omega) \quad ; \quad \beta \in (0, \infty] \quad (3)$$

where $e(\omega)$ is the energy density for the Hamiltonian (1) and $s(\omega)$ is the entropy density [13].

Notice that

$$e(\omega_\rho) = \text{Tr } \rho h_\rho \quad (4)$$

where

$$h_\rho = A + \frac{1}{2} B_\rho$$

$$B_\rho = \text{Tr}_2(1 \otimes \rho) B,$$

Tr_2 is the partial trace over the second space and

$$s(\omega_\rho) = - \text{Tr } \rho \log \rho. \quad (5)$$

DEFINITION II.1. — *i*) We call $\omega \in S$ globally thermodynamically stable for β (β - GTS) if

$$f_\beta(\omega) = \inf_{\sigma \in S} f_\beta(\sigma) \tag{6}$$

ii) $\omega \in S$ is called β - KMS state if for all local elements X of \mathcal{B}^∞ :

$$\lim_{\Lambda \rightarrow \infty} \beta \omega(X^*[H_\Lambda, X]) \geq \phi(\omega(X^*X), \omega(XX^*)) \tag{7}$$

where ϕ is the function from $[0, \infty)^2$ to $[0, \infty]$ given by:

$$\phi(u, v) = \begin{cases} u \ln u/v & \text{if } u + v > 0 \\ 0 & \text{if } u = v = 0 \end{cases}$$

The limit $\Lambda \rightarrow \infty$ is in the sense of taking any sequence of volumes which is increasing and absorbing.

iii) $\omega \in S$ is called a (strictly) stable β -KMS state if ω is a β -KMS-state and if for all elements $X \neq 0 \in \mathcal{B}$ and μ_ω almost all ρ :

$$\text{Tr} (\rho_X - \rho) \otimes (\rho_X - \rho) Q_\rho \geq 0 (> 0) \tag{8}$$

where

$$\rho_X = \frac{X\rho X^*}{\text{Tr} \rho X^*X}$$

$$Q_\rho = B + \beta^{-1} \psi(\rho \otimes 1, 1 \otimes \rho) P$$

and ψ is the function from $[0, \infty)^2$ to $[0, \infty]$ given by

$$\psi(u, v) = \begin{cases} \frac{\ln u/v}{u - v} & \text{if } u \neq v \\ \frac{1}{u} & \text{if } u = v. \end{cases} \tag{9}$$

LEMMA II.2. — If $\omega \in S$ is β -GTS with $\beta < \infty$ then for μ_ω almost all ρ :

- i*) $f_\beta(\omega) = f_\beta(\omega_\rho)$
- ii*) ρ^{-1} exists.

Proof. — *(i)* Follows trivially from $f_\beta(\omega) = \int d\mu_\omega(\rho) f_\beta(\omega_\rho)$ (see [13]);

ii) follows from *i*). Indeed suppose there exists a one dimensional projection operator R into the null space of ρ then, with $\sigma(\varepsilon) = (1 - \varepsilon)\rho + \varepsilon R$,

$$f(\omega_{\sigma(\varepsilon)}) - f_\beta(\omega_\rho) = \frac{1}{\beta} ([\varepsilon \ln \varepsilon + (1 - \varepsilon) \ln (1 - \varepsilon) - \varepsilon S(\omega_\rho)] + \varepsilon C_1 + \varepsilon^2 C_2$$

where C_1 and C_2 are constants, and this becomes negative for $\varepsilon > 0$ small enough, contradicting *i*).

LEMMA II.3. — If $T = 0$, then

$$f_\infty(\omega_{\sigma(\varepsilon, X)}) = f_\infty(\omega_\rho) + \varepsilon \text{Tr} (\rho_X - \rho) H_\rho + \frac{\varepsilon^2}{2} \text{Tr} (\rho_X - \rho) \otimes (\rho_X - \rho) B$$

If ρ^{-1} exists and $\beta < \infty$ then for each $X \in \mathcal{B}$ there exists a $\delta > 0$ such that for all $\varepsilon \in [0, \delta]$:

$$f_\beta(\omega_{\sigma(\varepsilon, X)}) = f_\beta(\omega_\rho) + \varepsilon \operatorname{Tr}(\rho_X - \rho) \left(H_\rho + \frac{1}{\beta} \ln \rho \right) + \frac{\varepsilon^2}{2} \operatorname{Tr}(\rho_X - \rho) \otimes (\rho_X - \rho) Q_\rho + \frac{\varepsilon^2}{3!} g(\varepsilon)$$

where $\sigma(\varepsilon, X) = (1 - \varepsilon)\rho + \varepsilon\rho_X$, $H_\rho = A + B_\rho$, $g(\varepsilon)$ is a bounded function of ε ; ρ_X , B_ρ and Q_ρ are as above.

Proof. — The case $T = 0$ is trivial. If ρ^{-1} exists, for each $X \in \mathcal{B}$ there exists a $\delta > 0$ such that for all $\varepsilon \in [0, \delta]$: $\sigma(\varepsilon, X) > 0$. Therefore the function $\varepsilon \in [0, \delta] \rightarrow f(\omega_{\sigma(\varepsilon, X)})$ is C^∞ . By the mean value theorem:

$$f_\beta(\omega_{\sigma(\varepsilon, X)}) = f_\beta(\omega_{\sigma(0, X)}) + \varepsilon \left[\frac{\partial f_\beta(\omega_{\sigma(\varepsilon, X)})}{\partial \varepsilon} \right]_{\varepsilon=0} + \frac{\varepsilon^2}{2!} \left[\frac{\partial^2 f_\beta(\omega_{\sigma(\varepsilon, X)})}{\partial \varepsilon^2} \right]_{\varepsilon=0} + \frac{\varepsilon^3}{3!} \left[\frac{\partial^3 f_\beta(\omega_{\sigma(\varepsilon', X)})}{\partial \varepsilon'^3} \right]_{\varepsilon' = \xi \in [0, \varepsilon]}$$

Remark that

$$f_\beta(\omega_{\sigma(0, X)}) = f_\beta(\omega_\rho)$$

and

$$\begin{aligned} \left. \frac{d}{d\varepsilon} e(\omega_{\sigma(\varepsilon, X)}) \right|_{\varepsilon=0} &= \operatorname{Tr}(\rho_X - \rho) H_\rho \\ \left. \frac{d^2}{d\varepsilon^2} e(\omega_{\sigma(\varepsilon, X)}) \right|_{\varepsilon=0} &= \operatorname{Tr}(\rho_X - \rho) \otimes (\rho_X - \rho) B \end{aligned}$$

To compute the derivatives of the entropy, the existence of $\sigma(\varepsilon, X)^{-1}$ guarantees the interchangeability of integration and derivation in the following calculation:

$$\begin{aligned} \frac{d}{d\varepsilon} \ln \sigma(\varepsilon, X) &= \frac{d}{d\varepsilon} \int_0^\infty d\lambda \left(\frac{1}{\lambda + 1} - \frac{1}{\lambda + \sigma(\varepsilon, X)} \right) \\ &= \int_0^\infty d\lambda \frac{1}{\lambda + \sigma(\varepsilon, X)} (\rho_X - \rho) \frac{1}{\lambda + \sigma(\varepsilon, X)} \end{aligned}$$

One gets

$$\left. \frac{d}{d\varepsilon} s(\omega_{\sigma(\varepsilon, X)}) \right|_{\varepsilon=0} = - \operatorname{Tr}(\rho_X - \rho) \ln \rho$$

and

$$\left. \frac{d^2}{d\varepsilon^2} s(\omega_{\sigma(\varepsilon, X)}) \right|_{\varepsilon=0} = - \operatorname{Tr}(\rho_X - \rho) \int_0^\infty d\lambda \frac{1}{\lambda + \rho} (\rho_X - \rho) \frac{1}{\lambda + \rho}.$$

To perform the λ -integration, consider the matrix units $(E_{ij} \mid i, j = 1, \dots, \dim \mathcal{H})$ in a basis (ϕ_j) diagonalizing the operator $\rho = \sum_i \rho_i E_{ii}$. Then

$$\operatorname{Tr}(\rho_X - \rho) \int_0^\infty d\lambda \frac{1}{\lambda + \rho} (\rho_X - \rho) \frac{1}{\lambda + \rho} = \sum_{i, j} \operatorname{Tr}(\rho_X - \rho) E_{ii} (\rho_X - \rho) E_{jj} \psi(\rho_i, \rho_j)$$

where ψ is defined in (9).

But

$$(\phi_k \otimes \phi_l, \psi(1 \otimes \rho, \rho \otimes 1)P\phi_i \otimes \phi_j) = \delta_{k,j}\delta_{l,i}\psi(\rho_i, \rho_j)$$

Hence

$$\frac{d^2}{d\varepsilon^2} s(\omega_{\sigma(\varepsilon, X)}) \Big|_{\varepsilon=0} = - \text{Tr} (\rho_X - \rho) \otimes (\rho_X - \rho) \psi(1 \otimes \rho, \rho \otimes 1)P.$$

Collecting the results of our calculations one gets the lemma. ■

Now we have the main result:

THEOREM II.4. — If $\omega \in S$ is β -GTS then ω is a stable β -KMS-state. Conversely, if $\omega \in S$ is a strictly stable β -KMS state then ω is relatively thermodynamically stable (i. e. local minimum).

Proof. — Suppose first that ω is β -GTS.

From Lemmas II.2 and II.3 it follows that μ_ω almost all ρ are of the form $\rho = ce^{-\beta H} \rho$, $c \in \mathbb{R}$, which in turn yields the β -KMS property by [7]. But for consistency we give an independent proof. We construct a one parameter symmetric locally normal perturbation ω_t of ω and construct an upper bound for $\liminf_{t \rightarrow 0^+} \frac{1}{t} (f_\beta(\omega_t) - f_\beta(\omega)) \geq 0$. By (2) $\omega = \int d\mu(\rho)\omega_\rho$ and define

the perturbed state by $\omega_t = \int d\mu(\rho)\omega_{\rho_t}$ where ρ_t will be defined as follows:

Let $X \in \mathcal{B}_\Lambda$, $\Lambda \subset Z^v$ and define γ by

$$\gamma(Y) = \frac{1}{2} (X^*[Y, X] + [X^*, Y]X), Y \in \mathcal{B}^\infty.$$

The map γ of \mathcal{B}^∞ in \mathcal{B}^∞ generates a norm continuous semigroup $(e^{t\gamma})_{t \geq 0}$ of positive unity preserving transformations of \mathcal{B}^∞ .

Let γ^* be the adjoint of γ , defined by

$$\text{Tr } Y_1 \gamma(Y_2) = \text{Tr } \gamma^*(Y_1) Y_2 \quad ; \quad Y_1, Y_2 \in \mathcal{B}^\infty$$

and then

$$\rho_t = \frac{1}{N(\Lambda)} \sum_{i \in \Lambda} \text{Tr}^{(i)} e^{t\gamma^*} \otimes_{i \in \Lambda} \rho$$

where $\text{Tr}^{(i)}$ stands for the partial trace over the space $\otimes_{j \in \Lambda \setminus \{i\}} \mathcal{H}_j$. Using the differentiability of the function $t \rightarrow f_\beta(\omega_t)$ at $t = 0$, and Lemma 6 of [2]:

$$\begin{aligned} \lim_{t \rightarrow 0^+} \frac{1}{t} (e(\omega_{\rho_t}) - e(\omega_\rho)) &= \frac{1}{N(\Lambda)} \lim_{N \rightarrow \infty} \omega_\rho(\gamma H_\Lambda) \\ \lim_{t \rightarrow 0^+} \frac{1}{t} (s(\omega_{\rho_t}) - s(\omega_\rho)) &= - \frac{1}{N(\Lambda)} \omega_\rho(\gamma \ln \otimes \rho) \\ &\geq \frac{1}{N(\Lambda)} \phi(\omega_\rho(X^*X), \omega_\rho(XX^*)) \end{aligned}$$

By Lebesgue dominated convergence and the joint convexity of the function $(u, v) \rightarrow \phi(u, v)$:

$$\begin{aligned} & \frac{1}{2} \lim_{\Lambda \rightarrow \infty} \omega(X^*[H_\Lambda, X] + [X^*, H_\Lambda]X) - \frac{1}{\beta} \phi(\omega(X^*X), \omega(XX^*)) \\ & \geq \liminf_{t \rightarrow 0^+} \frac{1}{t} [f_\beta(\omega_t) - f_\beta(\omega)] = \liminf_{t \rightarrow 0^+} \frac{1}{t} \int d\mu(\rho) [f_\beta(\omega_{\rho t}) - f_\beta(\omega_\rho)] \geq 0 \end{aligned}$$

We get the result if we prove that for all local $Y \in \mathcal{B}^\infty$: $\lim_{\Lambda \rightarrow \infty} \omega([Y, H_\Lambda]) = 0$.

But this follows again from GTS by now considering the map $\gamma = i[Y, \cdot]$. Hence any β -GTS is a β -KMS state. Furthermore it is also a stable β -KMS state. This follows from Lemma II.2 and 3. Conversely if ω is a strictly stable β -KMS-state then as ω is KMS it follows from [7] that μ_ω almost all ρ are of the form $\rho = Ce^{-\beta H_\rho}$, hence ρ^{-1} exists. The rest follows from Lemma II.3 and the fact that every density matrix on \mathcal{H} is obtained from ρ by $\rho_X = \frac{X\rho X^*}{\text{Tr } \rho X^*X}$ for a suitable $X \in \mathcal{B}$. ■

Remark that for the ground state $T = 0$ ($\beta = \infty$) one has the even more complete result. In this case GTS corresponds to minimal energy state, the KMS-property or ground state property [6] becomes:

for all local $X \in \mathcal{B}^\infty$

$$\lim_{\Lambda \rightarrow \infty} \omega(X^*[H_\Lambda, X]) \geq 0$$

and the stability becomes : for any density matrix $\sigma \in \mathcal{B}$:

$$\text{Tr} (\sigma - \rho)H_\rho \geq 0 ;$$

and if equality holds :

$$\text{Tr} (\sigma - \rho) \otimes (\sigma - \rho)B \geq 0$$

THEOREM II.5. — $\omega \in \mathcal{S}$ is a state of relative minimal energy if and only if ω is a stable ground state.

Proof. — This theorem follows from the previous one with the difference that we do not need the strict (strict inequality in (8)) stability, because the energy density is only of second order in the density matrices ρ . ■

Finally we want to make a number of remarks. It is known [7, 9] that for mean field models the KMS-condition is not equivalent with the variational principle of statistical mechanics, which was true for short range interactions e. g. for the case $T = 0$ see [6]. Nevertheless we recovered the relative minima by introducing the notion of stable-KMS-state which amounts to checking the positivity condition (8). First of all we warn the reader that this condition is not equivalent with the condition $Q_\rho \geq 0$, but that

it is strictly weaker. Furthermore condition (8) can be related to an upper bound of the Duhamel two point function, which is of course clear because it is a condition on the second derivative of free energy.

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