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Gibbs states of a quantum crystal: uniqueness by small particle mass

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Abstract A model of interacting quantum particles performing one-dimensional anharmonic oscillations around their unstable equilibrium positions, which form the lattice $\mathbb{Z}^d$, is considered. For this model, two statements describing its equilibrium properties are given. The first theorem states that there exists $m_* > 0$ such that for all values of the particle mass $m < m_*$, the set of tempered Euclidean Gibbs measures consists of exactly one element at all values of the temperature β^{-1}. This settles a problem that was open for a long time and is an essential improvement of a similar result proved before by the same authors [1] where the boundary m_* depended on β in such a way that $m_*(\beta) \to 0$ for $\beta \to +\infty$. The second theorem states that the two-point correlation function has an exponential decay if $m < m_*$. ***To cite this article: S. Albeverio et al., C. R. Acad. Sci. Paris, Ser. I 335 (2002) 693–698.***

États de Gibbs de crystaux quantiques: unicité dans le cas d'une petite masse

Résumé On considère un modèle de particules quantiques en intéraction effectuant des oscillations anharmoniques uni-dimensionelles autour de leur positions d'équilibre sur le réseau $\mathbb{Z}^d$. Pour ce modèle, nous énonçons deux résultats décrivant ses propriétés d'équilibre. Le premier théorème affirme l'existence de $m_* > 0$ tel que pour toutes les valeurs de la masse m de la particule inférieures à m_*, l'ensemble des mesures euclidiennes tempérées de Gibbs consiste en un seul élément, à toute température β^{-1}. Cela résoud un problème qui est resté ouvert pour longtemps et améliore essentiellement un résultat analogue obtenu par les mêmes auteurs, lorsque m_* dépendait de β de sorte que $m_*(\beta) \to 0$ si $\beta \to +\infty$. Le deuxième théorème dit que la fonction de corrélation a une décroissance exponentielle si $m < m_*$. ***Pour citer cet article : S. Albeverio et al., C. R. Acad. Sci. Paris, Ser. I 335 (2002) 693–698.***

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On considère un système de particules quantiques effectuant des oscillations uni-dimensionelles autour de leur positions d'équilibre sur le réseau $\mathbb{Z}^d$. L'Hamiltonien H de ce système est donné heuristiquement par

$$H = -\frac{J}{2}\sum_{\text{nn: } l,l'} \mathfrak{q}_l \mathfrak{q}_{l'} + \sum_l H_l^{(0)}, \quad J > 0,$$

où « nn » indique la condition $|l - l'| = 1$, $l, l' \in \mathbb{Z}^d$. L'Hamiltonien relatif à une particule de masse $m > 0$ est donné par

$$H_l^{(0)} = \frac{1}{2m}\mathfrak{p}_l^2 + \frac{1}{2}\mathfrak{q}_l^2 + V\left(\mathfrak{q}_l^2\right), \quad h \in \mathbb{R},$$

$$V(t) = at + b_2 t^2 + \cdots + b_r t^r, \quad a \in \mathbb{R},\ b_s \geqslant 0,\ b_r > 0,\ r \geqslant 2.$$

On considère les états du système donnés par des mesures de Gibbs tempérées sur l'espace (de dimension infini) des chemins périodiques de période β ($1/\beta$ étant la température).

On démontre que l'ensemble de toutes les mesures de Gibbs tempérées pures consiste d'un seul élément si $m < m_*$, où m_* est une constante indépendante de β (Théorème 2.1). Ceci donne donc l'unicité des mesures de Gibbs tempérées. Ce résultat précise considérablement un résultat d'unicité antérieur [1] où, au lieu de la borne m_* on avait seulement une borne $m_*(\beta) \to 0$, $\beta \to +\infty$. La démonstration du Théorème 2.1 est une conséquence du Théorème 2.2 qui affirme que la décroissance des « fonctions de Duhamel » (jouant le rôle des fonctions de corrélation) est exponentielle, si $m < m_*$, pour toutes les conditions au bord utilisées pour la construction des états de Gibbs et tous les β.

Les preuves des ces résultats utilisent les inégalités de corrélation, des estimations à priori des mesures de Gibbs et les propriétés spectrales des $H_l^{(0)}$, $l \in \mathbb{Z}^d$, étudiées, dans [3]

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1. The model and the Euclidean Gibbs states

We consider a system of interacting quantum particles performing one-dimensional anharmonic oscillations around their equilibrium positions which form a lattice $\mathbb{Z}^d$, $d \in \mathbb{N}$. The heuristic Hamiltonian of the model is

$$H = -\frac{J}{2}\sum_{\text{nn: } l,l'} \mathfrak{q}_l \mathfrak{q}_{l'} + \sum_l H_l^{(0)}, \quad J > 0, \tag{1}$$

where "nn" means that the sum is taken under the condition $|l - l| = 1$, $l, l' \in \mathbb{Z}^d$. The single-particle Hamiltonian $H_l^{(0)}$ has the form

$$H_l^{(0)} = \frac{1}{2m}\mathfrak{p}_l^2 + \frac{1}{2}\mathfrak{q}_l^2 + V(\mathfrak{q}_l^2), \quad h \in \mathbb{R}, \tag{2}$$

$$V(t) = at + b_2 t^2 + \cdots + b_r t^r, \quad a \in \mathbb{R},\ b_s \geqslant 0,\ b_r > 0,\ r \geqslant 2. \tag{3}$$

Here m denotes the particle mass. For $d \geqslant 3$ and large enough m, the system undergoes a phase transition [5], that means non-uniqueness of its Gibbs states. The same model was studied in our previous work [1], the present note gives an essential improvement of the result obtained there. Moreover, Theorem 2.1 below gives a complete answer on the problem of the role of quantum effects in phase transitions in such models, first considered in [9].

We take an approach in which Gibbs states are constructed as probability measures on path spaces. A detailed description of this *Euclidean* approach, full account of the results and extended bibliography may be found in the review article [2].

Let $\mathcal{X}_\beta$ denote the real Hilbert space $\mathrm{L}^2[0,\beta]$, $\beta > 0$, $\beta^{-1} = T$ is the temperature. By $\|\cdot\|_\beta$ and $(\cdot,\cdot)_\beta$ we denote the norm and inner product in $\mathcal{X}_\beta$. Set

$$S_\beta^{(m)} = [-m\Delta_\beta + 1]^{-1} : \mathcal{X}_\beta \to \mathcal{X}_\beta, \tag{4}$$

where Δ_β is the Laplacian with periodic boundary conditions. We denote by $\chi_\beta^{(m)}$ the Gaussian measure on $\mathcal{X}_\beta$, for which $S_\beta^{(m)}$ is the covariance operator. This measure is supported on the set of continuous periodic paths (Section 2.2 of [2])

$$\mathcal{C}_\beta = \bigl\{\omega \in \mathrm{C}[0,\beta] \mid \omega(0) = \omega(\beta)\bigr\} \subset \mathcal{X}_\beta.$$

For a finite box Λ, the set $\Omega_{\beta,\Lambda} = \{\omega_\Lambda = (\omega_l)_{l\in\Lambda} \mid \omega_l \in \mathcal{C}_\beta\}$ is a Banach space endowed with the supremum norm. The set of all configurations $\Omega_\beta = \mathcal{C}_\beta^{\mathbb{Z}^d}$ is endowed with the product topology. The set of *tempered configurations* is defined by

$$\Omega_\beta^{\mathrm{t}} = \left\{\omega \in \Omega_\beta \;\middle|\; \forall \delta > 0 : \sum_{l\in\mathbb{Z}^d} \mathrm{e}^{-\delta|l|}\|\omega_l\|_\beta < \infty\right\}, \tag{5}$$

where $|l|$ denotes the Euclidean distance. Given a box Λ, we set

$$\chi_{\beta,\Lambda}^{(m)}(\mathrm{d}\omega_\Lambda) = \bigotimes_{l\in\Lambda} \chi_\beta^{(m)}(\mathrm{d}\omega_l). \tag{6}$$

A conditional local Euclidean Gibbs measure is the following probability measure on $\Omega_{\beta,\Lambda}$

$$\nu_{\beta,\Lambda}(\mathrm{d}\omega_\Lambda|\xi) = \frac{1}{Z_{\beta,\Lambda}(\xi)} \exp\bigl(-E_{\beta,\Lambda}(\omega_\Lambda|\xi)\bigr)\chi_{\beta,\Lambda}^{(m)}(\mathrm{d}\omega_\Lambda), \quad \xi \in \Omega_\beta, \tag{7}$$

where

$$\begin{aligned} E_{\beta,\Lambda}(\omega_\Lambda|\xi) = {} & -\frac{J}{2}\sum_{nn:\, l,l'\in\Lambda}\int_0^\beta \omega_l(\tau)\omega_{l'}(\tau)\,\mathrm{d}\tau + \sum_{l\in\Lambda}\int_0^\beta V\bigl([\omega_l(\tau)]^2\bigr)\,\mathrm{d}\tau \\ & - J\sum_{\mathrm{nn}:\, l\in\Lambda,\ l'\in\Lambda^c}\int_0^\beta \omega_l(\tau)\xi_{l'}(\tau)\,\mathrm{d}\tau. \end{aligned} \tag{8}$$

For Λ and Borel subsets $B \subset \Omega_\beta$, we consider the probability kernels (see, e.g., [6])

$$\pi_{\beta,\Lambda}(B|\xi) = \int_{\Omega_{\beta,\Lambda}} \mathbf{1}_B(\omega_\Lambda \times \xi_{\Lambda^c})\nu_{\beta,\Lambda}(\mathrm{d}\omega_\Lambda|\xi). \tag{9}$$

DEFINITION 1.1. – The probability measure μ on Ω_β is said to be a Euclidean Gibbs measure at inverse temperature β if it satisfies the Dobrushin–Lanford–Ruelle (DLR) equation

$$\int_{\Omega_\beta} \pi_{\beta,\Lambda}(B|\omega)\mu(\mathrm{d}\omega) = \mu(B), \tag{10}$$

for all boxes Λ and all Borel subsets $B \subset \Omega_\beta$.

The set of all Euclidean Gibbs measures at a given β may contain measures with no physical relevance. Thus, we will restrict ourselves to the set $\mathcal{G}_\beta^{\mathrm{t}}$ of *tempered Euclidean Gibbs measures* consisting of all Euclidean Gibbs measures μ, such that $\mu(\Omega_\beta^{\mathrm{t}}) = 1$. By [4], $\mathcal{G}_\beta^{\mathrm{t}} \neq \emptyset$. One of the possible ways to study Euclidean Gibbs states of the model considered is the method of cluster expansions applied in [8] where, for small values of the mass, such expansions were shown to converge uniformly with respect to β. As a consequence, the existence of a Gibbs state and its clustering property were proved . At the same time, this convergence does not imply uniqueness because of the impossibility to control boundary conditions.

2. The results

THEOREM 2.1. – *There exists $m_* > 0$ such that, for all $m \in (0, m_*)$ and all temperatures, the set of tempered Euclidean Gibbs measures $\mathcal{G}^{\mathrm{t}}_\beta$ consists of exactly one element.*

In [1] we proved the uniqueness for $m \in (0, m_*(\beta))$ with $m_*(\beta) \to 0$ for $\beta \to +\infty$. The main progress in the above statement is that the upper bound m_* is independent of the temperature.

The proof of Theorem 2.1 is based on the following statement, which in itself gives an important information about the system we consider. Given $l, l' \in \Lambda$, $\tau, \tau' \in [0, \beta]$ and $\xi \in \Omega_\beta$, we set

$$K^{\Lambda}_{ll'}(\tau, \tau'|\xi) = \big\langle \omega_l(\tau)\omega_{l'}(\tau')\big\rangle_{\nu_{\beta,\Lambda}(\cdot|\xi)} - \big\langle \omega_l(\tau)\big\rangle_{\nu_{\beta,\Lambda}(\cdot|\xi)}\big\langle \omega_{l'}(\tau')\big\rangle_{\nu_{\beta,\Lambda}(\cdot|\xi)}, \tag{11}$$

where for a μ-integrable function f, we write

$$\langle f\rangle_\mu = \int f\,\mathrm{d}\mu.$$

Let $\Delta(m)$ denote the minimal distance between the eigenvalues of the single-particle Hamiltonian (3) but with the potential V replaced by

$$\widehat{V}(t) = at + 2^{-1}b_2t^2 + \cdots + 2^{1-r}b_rt^r.$$

We also set

$$\mathcal{K} = \left\{k = \frac{2\pi}{\beta}\kappa \;\middle|\; \kappa \in \mathbb{Z}\right\}, \qquad I(q) = 2J\sum_{j=1}^{d}\big(1 - \cos(q_j)\big), \quad q \in (-\pi, \pi]^d. \tag{12}$$

THEOREM 2.2. – *Let the parameters m and $\Delta(m)$, and the interaction intensity J satisfy the condition*

$$m\big[\Delta(m)\big]^2 > 2dJ. \tag{13}$$

Then, for any Λ and $\beta > 0$, for any $l, l' \in \Lambda$ and $\tau, \tau' \in [0, \beta]$, for arbitrary $\xi \in \Omega_\beta$, the correlation function (11) *obeys the estimate*

$$0 \leqslant K^{\Lambda}_{ll'}(\tau, \tau'|\xi) \leqslant \frac{1}{\beta(2\pi)^d}\sum_{k\in\mathcal{K}} \mathrm{e}^{\mathrm{i}k(\tau-\tau')}\int_{(-\pi,\pi]^d} \mathrm{e}^{\mathrm{i}(q,l-l')}\frac{\mathrm{d}q}{\Xi_\beta(k) + I(q)}, \tag{14}$$

where $\Xi_\beta(k)$ is a continuous function such that uniformly in $\beta > 0$

$$\Xi_\beta(k) > m\big[\Delta(m)\big]^2 + mk^2 - 2dJ, \quad k \in \mathcal{K}. \tag{15}$$

COROLLARY 2.3. – *Let* (13) *hold, then for the Duhamel function,*

$$D^{\Lambda}_{ll'}(\xi) \stackrel{\mathrm{def}}{=} \sup_{\tau\in[0,\beta]}\left\{\int_0^\beta K^{\Lambda}_{ll'}(\tau, \tau'|\xi)\,\mathrm{d}\tau'\right\} \leqslant C_1\exp\big(-\alpha|l - l'|\big), \quad \forall l, l' \in \Lambda, \tag{16}$$

with certain positive $C_1, \alpha > 0$, uniformly with respect to Λ and $\xi \in \Omega^{\mathrm{t}}_\beta$.

By [3], $m[\Delta(m)]^2 \sim C_2m^{-(r-1)/(r+1)}$ as $m \to 0$, hence (13) is satisfied for small enough m.

The rest of this Note contains a sketch of the proof of Theorem 2.1. Let $\mathcal{F}\mathcal{C}_{\mathrm{b}}(\Omega_\beta)$ (resp. $\mathcal{F}\mathcal{C}_{\mathrm{pb}}(\Omega_\beta)$) denote the set of bounded (resp. polynomially bounded) continuous cylinder functions $g : \Omega_\beta \to \mathbb{R}$. A net of measures μ_α on Ω_β *locally weakly converges* to a measure μ if $\forall g \in \mathcal{F}\mathcal{C}_{\mathrm{b}}(\Omega_\beta): \ \langle g\rangle_{\mu_\alpha} \to \langle g\rangle_\mu$.

For $\xi, \eta \in \Omega_\beta$, $\xi \geqslant \eta$ will mean $\xi_l(\tau) \geqslant \eta_l(\tau)$ for all $l \in \mathbb{Z}^d$, $\tau \in [0, \beta]$. A function $f : \Omega_\beta \to \mathbb{R}$ is called increasing if $f(\xi) \geqslant f(\eta)$ for $\xi \geqslant \eta$. A significant role in the proof is played by the FKG inequality, which, for the measures (7), was proved in Section 6 of [2]. By means of the FKG we prove the following

PROPOSITION 2.4. – *For every increasing $f \in \mathcal{F}\mathcal{C}_{\mathrm{pb}}(\Omega_\beta)$ and any $\xi, \eta \in \Omega_\beta$, $\xi \geqslant \eta$, implies*

$$\langle f \rangle_{\nu_{\beta,\Lambda}(\cdot|\xi)} \geqslant \langle f \rangle_{\nu_{\beta,\Lambda}(\cdot|\eta)}. \tag{17}$$

By means of a priori estimates for tempered Euclidean Gibbs measures [4] one proves the following

PROPOSITION 2.5. – *For any $\xi \in \Omega_\beta^{\mathrm{t}}$ and any sequence of boxes $\mathcal{L}$ which exhausts $\mathbb{Z}^d$, the sequence $\{\pi_{\beta,\Lambda}(\cdot|\xi)\}_{\mathcal{L}}$ is relatively compact in the topology of locally weak convergence. All its limiting points belong to $\mathcal{G}_\beta^{\mathrm{t}}$.*

These limiting points will be called *Minlos' states*. The set of such measures contains all pure tempered Gibbs measures (by Theorem 7.12, p. 122, [6]). Hence to prove the uniqueness one has to show that for an arbitrary f from a measure determining subset $\mathcal{F} \subset \mathcal{F}\mathcal{C}_{\mathrm{b}}(\Omega_\beta)$ and for any $\xi, \eta \in \Omega_\beta^{\mathrm{t}}$,

$$\langle f \rangle_{\nu_{\beta,\Lambda}(\cdot|\xi)} - \langle f \rangle_{\nu_{\beta,\Lambda}(\cdot|\eta)} \longrightarrow 0, \quad \Lambda \nearrow \mathbb{Z}^d. \tag{18}$$

As a measure determining subset $\mathcal{F}$, we choose the set consisting of the following functions. For each $f \in \mathcal{F}$, there exist $k \in \mathbb{N}$, $l_1, \ldots, l_k \in \mathbb{Z}^d$, $\tau_1, \ldots, \tau_k \in [0, \beta]$, $a_1, \ldots, a_k \in (0, +\infty)$ and a polynomial $p : \mathbb{R}^k \to \mathbb{R}$ such that

$$f(\omega) = p(\vartheta(\omega_{l_1}(\tau_1), a_1), \ldots, \vartheta(\omega_{l_k}(\tau_k), a_k)), \tag{19}$$

where for $x \in \mathbb{R}$,

$$\vartheta(x, a) \stackrel{\mathrm{def}}{=} \begin{cases} x & \text{if } |x| \leqslant a, \\ a \,\mathrm{sgn}(x) & \text{otherwise.} \end{cases}$$

Clearly, for very $f \in \mathcal{F}$, there exists $\lambda > 0$, such that the function

$$F(\omega) = \lambda \sum_{j=1}^{k} \omega_{l_j}(\tau_j) + \theta f(\omega), \quad F \in \mathcal{F}\mathcal{C}_{\mathrm{pb}}(\Omega_\beta), \tag{20}$$

is monotone for both $\theta = \pm 1$. Applying to this function Proposition 2.4 we obtain

$$\left| \langle f(\omega) \rangle_{\nu_{\beta,\Lambda}(\cdot|\xi)} - \langle f(\omega) \rangle_{\nu_{\beta,\Lambda}(\cdot|\eta)} \right| \leqslant \lambda \sum_{j=1}^{k} \left| \langle \omega_{l_j}(\tau_j) \rangle_{\nu_{\beta,\Lambda}(\cdot|\xi)} - \langle \omega_{l_j}(\tau_j) \rangle_{\nu_{\beta,\Lambda}(\cdot|\eta)} \right|,$$

which holds for any $\xi, \eta \in \Omega_\beta$. Thus, Theorem 2.1 will be proven by showing that

$$\langle \omega_{l_0}(\tau_0) \rangle_{\nu_{\beta,\Lambda}(\cdot|\xi)} - \langle \omega_{l_0}(\tau_0) \rangle_{\nu_{\beta,\Lambda}(\cdot|\eta)} \longrightarrow 0, \tag{21}$$

for all pairs $\xi, \eta \in \Omega_\beta^{\mathrm{t}}$. The idea of proving uniqueness by controlling just the first moments was inspired by the celebrated article [7]. To prove (21) we set

$$\psi(t|\Lambda) = \langle \omega_{l_0}(\tau_0) \rangle_{\nu_{\beta,\Lambda}(\cdot|\eta + t\zeta)}, \quad \zeta = \xi - \eta,\ t \in [0, 1]. \tag{22}$$

Then

$$\left| \langle \omega_{l_0}(\tau_0) \rangle_{\nu_{\beta,\Lambda}(\cdot|\xi)} - \langle \omega_{l_0}(\tau_0) \rangle_{\nu_{\beta,\Lambda}(\cdot|\eta)} \right| \leqslant \sup_{t \in [0,1]} \left| \psi'(t|\Lambda) \right|. \tag{23}$$

By (22) and (7), (8) one may compute the derivative ψ' explicitly

$$\psi'(t|\Lambda) = J \sum_{\mathrm{nn:}\ l \in \Lambda, l' \in \Lambda^c} \int_0^\beta K_{l l_0}^{\Lambda}(\tau, \tau_0|\eta + t\zeta) \zeta_{l'}(\tau)\, \mathrm{d}\tau,$$

where $K^{\Lambda}_{ll_0}$ is given by (11). After some calculations we arrive at

$$\left|\psi'(t|\Lambda)\right| \leqslant A(\beta, J) \sum_{\text{nn: } l\in\Lambda, l'\in\Lambda^c} \left[D^{\Lambda}_{ll_0}(\eta + t\zeta)\right]^{1/2} \|\zeta_{l'}\|_{\beta},$$

where $A(\beta, J)$ is independent of Λ. Taking into account (16) and the fact that $\zeta \in \Omega^{\mathrm{t}}_{\beta}$, we obtain (21).

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