Gibbs States of Interacting Systems of Quantum Anharmonic Oscillators *

Yuri Kozitsky (jkozil@golem.umcs.lublin.pl)
Instytut Matematyki, Uniwersytet Marii Curie-Skłodowskiej, Lublin 20-031 Poland

Tatiana Pasurek (tpasurek@math.uni-bielefeld.de)
Fakultät für Mathematik und Forschungszentrum BiBoS, Universität Bielefeld, D-33615 Bielefeld, Germany

Abstract. A complete description of the equilibrium thermodynamic properties of an infinite system of interacting ν-dimensional quantum anharmonic oscillators is given. The oscillators are indexed by the elements of a countable set $\mathbb{L} \subset \mathbb{R}^d$, possibly irregular; the anharmonic potentials vary from site to site. The description is based on the representation of the Gibbs states in terms of path measures. In particular, it is stated that (a) the set of Gibbs measures $\mathcal{G}^{\rm t}$ is non-void and compact; (b) every $\mu \in \mathcal{G}^{\rm t}$ obeys exponential integrability estimates, the same for the whole $\mathcal{G}^{\rm t}$; (c) every $\mu \in \mathcal{G}^{\rm t}$ has a Lebowitz-Presutti type support; (d) $|\mathcal{G}^{\rm t}| = 1$ at high temperatures. In the case of $\nu = 1$ and attractive interaction, the existence of phase transitions and uniqueness of Gibbs measures due to quantum effects are also described. Finally, it is shown that $|\mathcal{G}^{\rm t}| = 1$ at a non-zero external field.

Keywords: Tempered configurations, temperature loops, Gibbs specification, DLR equation, phase transitions, quantum anharmonic crystal, quantum effects.

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1. Introduction and Setup

The quantum anharmonic oscillator is a mathematical model of a localized quantum particle moving in a potential field with possibly multiple minima. Infinite systems of interacting quantum anharmonic oscillators possess interesting properties connected with the ordering caused by the interaction, as well as with quantum stabilization competing the ordering. Most of the systems of this kind are related with solids, such as ionic crystals containing localized light particles oscillating in the field created by heavy ionic complexes, or quantum crystals consisting entirely of such particles. For instance, a potential field with multiple minima is seen by a helium atom located at the center of the crystal cell in bcc helium [21]. The same situation exists in other quantum crystals, He, H_2 and to some extent Ne. An example of the ionic crystal with

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localized quantum particles moving in a double-well potential field is a KDP-type ferroelectric with hydrogen bounds, in which such particles are protons or deuterons performing one-dimensional oscillations along the bounds. In this case the particle carries electric charge and its displacement produces dipole moment, that should be reflected in the choice of the inter-particle interaction. It is believed that structural phase transitions in such ferroelectrics are triggered by ordering of protons [13, 31, 32]. Another relevant physical object is a system of light atoms, like Li, doped into ionic crystals, like KCl, where the quantum particles are not necessarily regularly distributed and the anharmonic potential may vary from site to site. At last, quantum anharmonic oscillators are used as parts of the models describing interaction of vibrating quantum particles with a radiation (photon) field [18, 27] or strong electron-electron correlations caused by the interaction of electrons with vibrating ions, responsible for such interesting phenomena as superconductivity, charge density waves etc, see [16]. Thereby, systems of quantum anharmonic oscillators with possibly irregular properties are quite important objects of theoretical physics and their rigorous description is still a challenging mathematical task.

The model we consider has the following heuristic Hamiltonian

$$H = -\frac{1}{2}\sum_{\ell,\ell'} J_{\ell\ell'}(q_\ell, q_{\ell'}) + \sum_{\ell} H_\ell, \tag{1}$$

where the sums run through a countable set $\mathbb{L} \subset \mathbb{R}^d$. This set is equipped with the Euclidean distance $|\ell - \ell'|$. We suppose that

$$\sup_{\ell\in\mathbb{L}} \sum_{\ell'\in\mathbb{L}} \frac{1}{(1+|\ell-\ell'|)^{d+\epsilon}} < \infty, \tag{2}$$

for some $\epsilon > 0$. This is a kind of regularity of $\mathbb{L}$, which in particular means that big amounts of the elements of $\mathbb{L}$ cannot concentrate in subsets of $\mathbb{R}^d$ of small volume. A regular case of $\mathbb{L}$ is a lattice, which for simplicity is supposed to be $\mathbb{Z}^d$. In this case the model is *a quantum anharmonic crystal.* The displacement q_ℓ is a ν-dimensional vector. The interaction term in (1) is of dipole-dipole type. By $(\cdot,\cdot)$ and $|\cdot|$ we denote the scalar product and norm in the Euclidean spaces $\mathbb{R}^\nu$, $\mathbb{R}^d$. The Hamiltonian

$$H_\ell = H_\ell^{\rm har} + V_\ell(q_\ell) \ \stackrel{\rm def}{=}\ \frac{1}{2m}|p_\ell|^2 + \frac{a}{2}|q_\ell|^2 + V_\ell(q_\ell), \quad a > 0, \tag{3}$$

describes an isolated anharmonic oscillator of mass m and momentum p_ℓ. The Hamiltonian $H_\ell^{\rm har}$ corresponds to a quantum harmonic oscillator of rigidity a. The anharmonic terms V_ℓ, which may vary from site to site, are supposed to obey certain uniform bounds. We do not assume that the interaction intensities $J_{\ell\ell'}$ possess special properties like translation invariance in case $\mathbb{L} = \mathbb{Z}^d$ or has finite range. Therefore, our model can describe also systems with spacial irregularities like impurities or the ones with random components.

A complete description of the equilibrium thermodynamic properties of infinite-particle systems may be made by constructing their Gibbs states. The Gibbs states of a quantum model are defined as positive normalized functionals on algebras of observables satisfying the Kubo-Martin-Schwinger (KMS) condition [14], which reflects the consistency between the dynamic and thermodynamic properties of the model proper to the thermodynamic equilibrium. For a subsystem located in a finite $\Lambda \subset \mathbb{L}$ described by the local Hamiltonian H_Λ, the KMS condition is formulated by means of the unitary operators $\exp(\imath t H_\Lambda)$, $t \in \mathbb{R}$, which are used to describe the evolution of the observables and hence determine the dynamics of the subsystem. To describe the dynamics of the whole model one takes the infinite-volume limit of $\exp(\imath t H_\Lambda)$. For our model, such limits do not exist; thus, the time automorphisms describing the dynamics of the whole infinite model cannot be defined and the corresponding KMS conditions cannot be formulated. This is a fundamental problem and actually there is no canonical way to define Gibbs states, and hence to describe thermodynamic properties of such models. In this situation one has to develop another approach, adequate for describing relevant physical properties. In [1], it was initiated an approach based on the fact that the local Hamiltonians H_Λ generate stochastic processes. Then the description of the local Gibbs states, based on the properties of the semi-groups $\exp(-\tau H_\Lambda)$, $\tau > 0$, is translated into 'a probabilistic language', which opens the possibility to apply here concepts and techniques from this domain. In this language our model is a system of infinite-dimensional 'spins' ω_ℓ, $\ell \in \mathbb{L}$, being continuous functions $\omega_\ell : [0, \beta] \to \mathbb{R}^\nu$, i.e., paths, such that $\omega(0) = \omega(\beta)$, where $\beta^{-1} = T > 0$ is temperature. Each 'spin' is described by the path measure of the β-periodic Ornstein-Uhlenbeck process corresponding to $H_\ell^{\rm har}$, multiplied by a density obtained from the anharmonic term V_ℓ by means of the Feynman-Kac formula. Finite subsystems are associated with conditional probability measures, which through the Dobrushin-Lanford-Ruelle (DLR) formalism determine the set of Gibbs measures $\mathcal{G}^{\rm t}$. This approach is called Euclidean due to the conceptual analogy with the Euclidean quantum field theory. Among its achievements there is the settlement in [4, 5] of a long standing problem of the influence of quantum effects on structural phase transitions in quantum anharmonic crystals, first discussed in [29].

In the present letter, we give a complete description of the set $\mathcal{G}^{\rm t}$ for the model (1), and hence finalize the development of the Euclidean approach for such models. Our results fall into two groups of theorems. The first group describes the general case where $J_{\ell\ell'}$ and V_ℓ obey natural stability conditions only. We state that: $\mathcal{G}^{\rm t}$ is non-void and compact (Theorem 3.1); the elements of $\mathcal{G}^{\rm t}$ obey exponential integrability estimates (Theorem 3.2) and have a Lebowitz-Presutti type support (Theorem 3.3); $\mathcal{G}^{\rm t}$ contains exactly one element at high temperatures (Theorem 3.4). The second group of theorems describes the case of $\nu = 1$, even V_ℓ, and $J_{\ell\ell'} \geq 0$. Here we employ the FKG order and show that the set $\mathcal{G}^{\rm t}$ has maximal and minimal elements (Theorem 3.5). Then under natural additional conditions on V_ℓ we state (Theorem 3.6) that for $d \geq 3$, $|\mathcal{G}^{\rm t}| > 1$ at big enough β, i.e., the model undergoes a phase transition; and that $|\mathcal{G}^{\rm t}| = 1$ at all β if a quantum stabilization condition is satisfied (Theorem 3.7). Finally, under a more restrictive condition on V_ℓ we show that $|\mathcal{G}^{\rm t}| = 1$ at non-zero external field and all β (Theorem 3.8).

The proof of these theorems, which will be published in a separate article[1], heavily employs probabilistic methods and is far beyond the scope of this letter. Here we are not even discussing its scheme. Instead, in Section 2 we give a detailed introduction into the Euclidean method in the context of our model. A comparison with the corresponding results known in the literature is given at the very end of the letter.

2. Gibbs States

2.1. The Model and its Local Gibbs States

We assume that the anharmonic potentials V_ℓ are continuous functions $\mathbb{R}^\nu \to \mathbb{R}$, such that for all $\ell \in \mathbb{L}$ and $x \in \mathbb{R}^\nu$,

$$A_V |x|^{2r} + B_V \leq V_\ell(x) \leq V(x), \tag{4}$$

with a certain continuous $V : \mathbb{R}^\nu \to \mathbb{R}$ and constants $r > 1$, $A_V > 0$, and $B_V \in \mathbb{R}$. An example of V_ℓ to bear in mind is

$$V_\ell(x) = \sum_{s=1}^{r} b_\ell^{(s)} |x|^{2s} - (h, x), \quad b_\ell^{(s)} \in \mathbb{R}, \quad r \geq 2, \tag{5}$$

in which $h \in \mathbb{R}^\nu$ is an external field and the coefficient $b_\ell^{(s)}$ are confined to certain intervals such that both estimates (4) hold.

[1] A preprint version appeared as [25].

For the inter-particle interaction intensities $J_{\ell\ell'}$, we assume that

$$J_{\ell\ell'} = J_{\ell'\ell}, \quad J_{\ell\ell} = 0, \quad \text{and} \quad \hat{J}_0 \stackrel{\text{def}}{=} \sup_{\ell} \sum_{\ell'} |J_{\ell\ell'}| < \infty. \tag{6}$$

The model (1) is called ferroelectric[2] if $J_{\ell\ell'} \geq 0$ for all $\ell, \ell' \in \mathbb{L}$. By Λ we denote subsets of $\mathbb{L}$; for a non-void finite subset, we write $\Lambda \Subset \mathbb{L}$. If we say that something holds for all ℓ, we mean it holds for all $\ell \in \mathbb{L}$; sums like $\sum_{\ell}$ mean $\sum_{\ell \in \mathbb{L}}$.

The heuristic Hamiltonian (1) has no direct mathematical meaning and is 'represented' by local Hamiltonians

$$H_\Lambda = -\frac{1}{2} \sum_{\ell, \ell' \in \Lambda} J_{\ell\ell'}(q_\ell, q_{\ell'}) + \sum_{\ell \in \Lambda} H_\ell, \quad \Lambda \Subset \mathbb{L}, \tag{7}$$

which by the above assumptions are essentially self-adjoint and lower bounded operators acting in the physical Hilbert spaces $\mathcal{H}_\Lambda = L^2(\mathbb{R}^{\nu|\Lambda|})$. For every $\beta > 0$,

$$Z_\Lambda \stackrel{\text{def}}{=} \text{trace}[\exp(-\beta H_\Lambda)] < \infty; \tag{8}$$

thus, one can introduce the local Gibbs state

$$A \mapsto \varrho_\Lambda(A) = \text{trace}[A \exp(-\beta H_\Lambda)]/Z_\Lambda, \tag{9}$$

which is a positive normal functional on the algebras $\mathfrak{C}_\Lambda$ of all bounded linear operators on $\mathcal{H}_\Lambda$. The dynamics of the subsytem in Λ is described by the local time automorphisms

$$A \mapsto \mathfrak{a}_t^\Lambda(A) = \exp\left(\imath t H_\Lambda\right) A \exp\left(-\imath t H_\Lambda\right), \quad t \in \mathbb{R}, \quad \Lambda \Subset \mathbb{L}. \tag{10}$$

Let $\mathfrak{M}_\Lambda^{\text{cont}}$ be the algebra of all multiplication operators by bounded continuous functions $F \in C_{\text{b}}(\mathbb{R}^{\nu|\Lambda|})$. One can prove, see [24], that the linear span of the operators $\mathfrak{a}_{t_1}^\Lambda(F_1) \cdots \mathfrak{a}_{t_n}^\Lambda(F_n)$ with all possible choices of $n \in \mathbb{N}$, $t_1, \ldots, t_n \in \mathbb{R}$, and $F_1, \ldots, F_n \in \mathfrak{M}_\Lambda^{\text{cont}}$, is dense in $\mathfrak{C}_\Lambda$ in the σ-weak topology. Since normal functionals are σ-weakly continuous, the state (9) is fully determined by its values on the mentioned products, i.e., by the local Green functions

$$G_{F_1,\ldots,F_n}^\Lambda(t_1, \ldots, t_n) = \varrho_\Lambda \left[\mathfrak{a}_{t_1}^\Lambda(F_1) \cdots \mathfrak{a}_{t_n}^\Lambda(F_n)\right]. \tag{11}$$

Each such a function can be looked upon, see [1, 3, 12], as the restrictions of a function $G_{F_1,\ldots,F_n}^\Lambda$ analytic on the domain

$$\mathcal{D}_\beta^n = \{(t_1, \ldots, t_n) \in \mathbb{C}^n \mid 0 < \Im(t_1) < \cdots < \Im(t_n) < \beta\}, \tag{12}$$

[2] Usually such a model is called 'ferromagnetic'; we adopt the above terminology in view of the ferroelectric interpretation mentioned in Introduction.

and continuous on its closure $\bar{\mathcal{D}}^n_\beta$. For every $n \in \mathbb{N}$, the subset

$$\{(t_1, \ldots, t_n) \in \mathcal{D}^n_\beta \mid \Re(t_1) = \ldots = \Re(t_n) = 0\},$$

is an inner set of uniqueness for functions analytic on $\mathcal{D}^n_\beta$, see pages 101 and 325 in [30]. This means that the Matsubara functions

$$\Gamma^\Lambda_{F_1,\ldots,F_n}(\tau_1, \ldots, \tau_n) \stackrel{\mathrm{def}}{=} G^\Lambda_{F_1,\ldots,F_n}(\imath\tau_1, \ldots, \imath\tau_n), \tag{13}$$

defined for $0 \leq \tau_1 \leq \cdots \leq \tau_n \leq \beta$, uniquely determine the corresponding Green functions and hence the states ϱ_Λ. They have the property

$$\Gamma^\Lambda_{F_1,\ldots,F_n}(\tau_1 + \vartheta, \ldots, \tau_n + \vartheta) = \Gamma^\Lambda_{F_1,\ldots,F_n}(\tau_1, \ldots, \tau_n),$$

where addition is modulo β. This periodicity and the analyticity of the Green functions imply the KMS property of the state ϱ_Λ [1, 12, 19]. As was mentioned above, one cannot get the thermodynamic limits of the automorphisms (10), which would be used to define the global KMS states. To overcome this difficulty the states of the whole model are constructed as probability measures on path spaces, called Euclidean Gibbs states or Euclidean Gibbs measures. For every $\Lambda \Subset \mathbb{L}$, the semigroup $\exp(-\tau H_\Lambda)$, $\tau \in [0, \beta]$, generates a β-periodic Markov process, [19, 20], associated with the probability measure μ_Λ such that the functions (13) are the moments of μ_Λ, which fully determines the local state (9). By means of such measures one constructs the set of Euclidean Gibbs states $\mathcal{G}^{\mathrm{t}}$.

2.2. Euclidean Gibbs States

As was mentioned above, the 'spins' are continuous functions $\omega_\ell : [0, \beta] \to \mathbb{R}^\nu$, taking equal values at the endpoints (temperature loops). Thus, one can define them on the circle $S_\beta \cong [0, \beta]$. As single spin spaces we use the standard Banach spaces

$$C_\beta \stackrel{\mathrm{def}}{=} C(S_\beta \to \mathbb{R}^\nu), \qquad C^\sigma_\beta \stackrel{\mathrm{def}}{=} C^\sigma(S_\beta \to \mathbb{R}^\nu), \quad \sigma \in (0, 1/2),$$

of all continuous and Hölder-continuous functions $\omega_\ell : S_\beta \to \mathbb{R}^\nu$, equipped respectively with the supremum norm $|\omega_\ell|_{C_\beta}$ and with the Hölder norm

$$|\omega_\ell|_{C^\sigma_\beta} = |\omega_\ell|_{C_\beta} + \sup_{\tau,\tau' \in S_\beta,\ \tau \neq \tau'} \frac{|\omega_\ell(\tau) - \omega_\ell(\tau')|}{|\tau - \tau'|^\sigma_\beta}. \tag{14}$$

We also use the Hilbert space $L^2_\beta = L^2(S_\beta \to \mathbb{R}^\nu, \mathrm{d}\tau)$, with the inner product and norm $(\cdot, \cdot)_{L^2_\beta}$, $|\cdot|_{L^2_\beta}$. By $\mathcal{B}(C_\beta)$, $\mathcal{B}(L^2_\beta)$ we denote the corresponding Borel σ-algebras. In a standard way, see page 21 of [28], one proves that

$$C_\beta \in \mathcal{B}(L^2_\beta) \quad \text{and} \quad \mathcal{B}(C_\beta) = \mathcal{B}(L^2_\beta) \cap C_\beta. \tag{15}$$

Given $\Lambda \subseteq \mathbb{L}$, we set

$$\Omega_\Lambda = \{\omega_\Lambda = (\omega_\ell)_{\ell\in\Lambda} \mid \omega_\ell \in C_\beta\}, \quad \Omega = \Omega_{\mathbb{L}} = \{\omega = (\omega_\ell)_{\ell\in\mathbb{L}} \mid \omega_\ell \in C_\beta\}.$$

These path spaces are equipped with the product topology and with the Borel σ-algebras $\mathcal{B}(\Omega_\Lambda)$. Thereby, each Ω_Λ is a complete separable metric space, its elements are called configurations in Λ. For $\Lambda \subset \Lambda'$, we write $\omega_{\Lambda'} = \omega_\Lambda \times \omega_{\Lambda'\setminus\Lambda}$, which defines an embedding $\Omega_\Lambda \hookrightarrow \Omega_{\Lambda'}$ by identifying $\omega_\Lambda \in \Omega_\Lambda$ with $\omega_\Lambda \times 0_{\Lambda'\setminus\Lambda} \in \Omega_{\Lambda'}$. By $\mathcal{P}(\Omega)$ we denote the set of all probability measures on $(\Omega, \mathcal{B}(\Omega))$.

The harmonic part of (3) defines the semigroup $\exp(-\tau H^{\rm har}_\ell)$, $\tau \in [0,\beta]$, and hence the β-periodic Ornstein-Uhlenbeck process [20]. Its realization on $(C_\beta, \mathcal{B}(C_\beta))$ is described by the Gaussian measure χ, which we introduce as follows. In L^2_β we define the Laplace-Beltrami type operator

$$A = \left(-m\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + a\right) \otimes \mathbf{I}, \quad \mathbf{I} = \mathrm{Id} : \mathbb{R}^\nu \to \mathbb{R}^\nu,$$

such that A^{-1} is of trace class. Therefore, the Fourier transformation

$$\int_{L^2_\beta} \exp[\imath(\phi, \upsilon)_{L^2_\beta}]\chi(\mathrm{d}\upsilon) = \exp\left\{-\frac{1}{2}(A^{-1}\phi, \phi)_{L^2_\beta}\right\}, \quad \phi \in L^2_\beta. \tag{16}$$

defines a Gaussian measure χ on $(L^2_\beta, \mathcal{B}(L^2_\beta))$, possessing the property

$$\chi(C^\sigma_\beta) = 1, \quad \text{for all } \sigma \in (0, 1/2). \tag{17}$$

This yields $\chi(C_\beta) = 1$; hence, by (15) we redefine χ as a probability measure on $(C_\beta, \mathcal{B}(C_\beta))$. By standard arguments (Fernique's theorem), it follows from (17) that for every $\sigma \in (0, 1/2)$, there exists $\lambda_\sigma > 0$ such that

$$\int_{L^2_\beta} \exp\left(\lambda_\sigma |\upsilon|^2_{C^\sigma_\beta}\right) \chi(\mathrm{d}\upsilon) < \infty. \tag{18}$$

For $\Lambda \Subset \mathbb{L}$, we set

$$\chi_\Lambda(\mathrm{d}\omega_\Lambda) = \prod_{\ell\in\Lambda} \chi(\mathrm{d}\omega_\ell), \tag{19}$$

and

$$I_\Lambda(\omega_\Lambda) = -\frac{1}{2}\sum_{\ell,\ell'\in\Lambda} J_{\ell\ell'}(\omega_\ell, \omega_{\ell'})_{L^2_\beta} + \sum_{\ell\in\Lambda}\int_0^\beta V_\ell(\omega_\ell(\tau))\mathrm{d}\tau. \tag{20}$$

The latter is the energy functional describing the system of interacting paths ω_ℓ, $\ell \in \Lambda$. Thereby, the measure μ_Λ is

$$\mu_\Lambda(\mathrm{d}\omega_\Lambda) = \exp\left\{-I_\Lambda(\omega_\Lambda)\right\}\chi_\Lambda(\mathrm{d}\omega_\Lambda)/Z_\Lambda, \tag{21}$$

where the partition function Z_Λ is given by (8). Here it serves as a normalizing factor. In what follows, the scheme described above establishes a one-to-one correspondence between the local Gibbs states (9) and the local Euclidean Gibbs measures (21). The Euclidean Gibbs measures corresponding to the whole system are defined in the DLR approach, see [17]. To introduce them we need functions $f : \Omega_\Lambda \to \mathbb{R}$ with infinite Λ, including the Ω itself. In particular, we will use the energy functional

$$I_\Lambda(\omega|\xi) = I_\Lambda(\omega_\Lambda) - \sum_{\ell\in\Lambda,\ \ell'\in\Lambda^c} J_{\ell\ell'}(\omega_\ell, \xi_{\ell'})_{L^2_\beta}, \quad \omega \in \Omega, \tag{22}$$

describing the interaction of the paths inside $\Lambda \Subset \mathbb{L}$ between themselves and with the configuration $\xi \in \Omega$ fixed outside Λ. The second term here makes sense for all $\xi \in \Omega$ only if $J_{\ell\ell'}$ has finite range. Otherwise, one has to restrict ξ to be a tempered configuration. In one or another way, tempered configurations appear in all problems involving unbounded spins [11, 26]. We impose the weakest possible restrictions of this kind. To introduce them we use weights, which by definition are the maps $w_\alpha : \mathbb{L}^2 \to (0, +\infty)$, $\alpha \in \mathcal{I} = (\underline{\alpha}, \overline{\alpha}) \subseteq (0, +\infty)$ obeying the conditions

(a) for any $\alpha \in \mathcal{I}$ and ℓ, $\quad w_\alpha(\ell, \ell) = 1$;

(b) for any $\alpha \in \mathcal{I}$ and ℓ_1, ℓ_2, ℓ_3,

$$w_\alpha(\ell_1, \ell_2) \cdot w_\alpha(\ell_2, \ell_3) \leq w_\alpha(\ell_1, \ell_3) \quad \textit{(triangle inequality)}; \tag{23}$$

(c) for any $\alpha, \alpha' \in \mathcal{I}$, such that $\alpha < \alpha'$, and arbitrary ℓ, ℓ',

$$w_{\alpha'}(\ell, \ell') \leq w_\alpha(\ell, \ell'), \qquad \lim_{|\ell-\ell'|\to+\infty} w_{\alpha'}(\ell, \ell')/w_\alpha(\ell, \ell') = 0. \tag{24}$$

The concrete choice of the weights depends on the decay of $J_{\ell\ell'}$, which thus will be subject to the following

ASSUMPTION 2.1. *For all $\alpha \in \mathcal{I}$,*

$$\sup_\ell \sum_{\ell'} \log(1 + |\ell - \ell'|) \cdot w_\alpha(\ell, \ell') < \infty; \tag{25}$$

$$\sup_\ell \sum_{\ell'} |J_{\ell\ell'}| \cdot \left[w_\alpha(\ell, \ell')\right]^{-1} < \infty. \tag{26}$$

One observes that (25) and (26) are competitive. Let us consider some concrete examples. Suppose that

$$\sup_{\ell} \sum_{\ell'} |J_{\ell\ell'}| \cdot \exp\left(\alpha|\ell - \ell'|\right) < \infty, \quad \text{with a certain } \alpha > 0. \tag{27}$$

The supremum of such α (possibly $+\infty$) is denoted by $\overline{\alpha}$. Then we set

$$\mathcal{I} = (0, \overline{\alpha}), \quad w_{\alpha}(\ell, \ell') = \exp\left(-\alpha|\ell - \ell'|\right). \tag{28}$$

If (27) does not hold for any positive α, we assume that

$$\sup_{\ell} \sum_{\ell'} |J_{\ell\ell'}| \cdot \left(1 + |\ell - \ell'|\right)^{\alpha d} < \infty, \quad \text{with a certain } \alpha > 1, \tag{29}$$

and set $\overline{\alpha}$ to be the supremum of α obeying (29). Thereby,

$$\mathcal{I} = (1, \overline{\alpha}), \quad w_{\alpha}(\ell, \ell') = \left(1 + \varepsilon|\ell - \ell'|\right)^{-\alpha d}, \quad \alpha \in \mathcal{I}, \tag{30}$$

where $\varepsilon > 0$ is a certain fixed parameter, c.f., (2).

For a certain $\underline{\ell}$, we introduce

$$\Omega_{\alpha} = \left\{ \omega \in \Omega \,\middle|\, \|\omega\|_{\alpha} \stackrel{\text{def}}{=} \left[\sum_{\ell} |\omega_{\ell}|^2_{L^2_{\beta}} w_{\alpha}(\underline{\ell}, \ell) \right]^{1/2} < \infty \right\}. \tag{31}$$

Equipped with the metric

$$\rho_{\alpha}(\omega, \omega') = \|\omega - \omega'\|_{\alpha} + \sum_{\ell} 2^{-|\underline{\ell} - \ell|} \cdot \frac{|\omega_{\ell} - \omega'_{\ell}|_{C_{\beta}}}{1 + |\omega_{\ell} - \omega'_{\ell}|_{C_{\beta}}}, \tag{32}$$

it becomes a complete separable metric space. The set of tempered configurations is then defined to be

$$\Omega^{\rm t} = \bigcap_{\alpha \in \mathcal{I}} \Omega_{\alpha}. \tag{33}$$

In the projective limit topology $\Omega^{\rm t}$ becomes a complete separable metric space as well. Clearly, the topologies of the spaces Ω_{α}, $\Omega^{\rm t}$ are independent of the choice of $\underline{\ell}$. By construction, for any $\alpha \in \mathcal{I}$, we have continuous dense embeddings $\Omega^{\rm t} \hookrightarrow \Omega_{\alpha} \hookrightarrow \Omega$, which yields that $\Omega_{\alpha}, \Omega^{\rm t} \in \mathcal{B}(\Omega)$ and the Borel σ-algebras of all these spaces coincide with the σ-algebras induced on them by $\mathcal{B}(\Omega)$.

By standard methods, one can prove that for every $\alpha \in \mathcal{I}$ and $\Lambda \Subset \mathbb{L}$, the map $\Omega_{\alpha} \times \Omega_{\alpha} \ni (\omega, \xi) \mapsto I_{\Lambda}(\omega|\xi)$ is continuous. Furthermore, for every ball $B_{\alpha}(r) = \{\omega \in \Omega_{\alpha} \mid \rho_{\alpha}(0, \omega) < r\}$, $r > 0$, one has

$$\inf_{\omega \in \Omega,\ \xi \in B_{\alpha}(r)} I_{\Lambda}(\omega|\xi) > -\infty, \qquad \sup_{\omega, \xi \in B_{\alpha}(r)} |I_{\Lambda}(\omega|\xi)| < +\infty.$$

Therefore, for $\Lambda \Subset \mathbb{L}$ and $\xi \in \Omega^{\rm t}$, the partition function

$$Z_\Lambda(\xi) = \int_{\Omega_\Lambda} \exp\left[-I_\Lambda(\omega_\Lambda \times 0_{\Lambda^c}|\xi)\right] \chi_\Lambda(\mathrm{d}\omega_\Lambda) \tag{34}$$

is continuous and for any $r > 0$, $\inf_{\xi \in B_\alpha(r)} Z_\Lambda(\xi) > 0$. Thus, one can define

$$\pi_\Lambda(B|\xi) = \frac{1}{Z_\Lambda(\xi)} \int_{\Omega_\Lambda} \exp\left[-I_\Lambda(\omega_\Lambda \times 0_{\Lambda^c}|\xi)\right] \mathbb{I}_B(\omega_\Lambda \times \xi_{\Lambda^c}) \chi_\Lambda(\mathrm{d}\omega_\Lambda), \tag{35}$$

where $\xi \in \Omega^{\rm t}$, $\Lambda \Subset \mathbb{L}$, $B \in \mathcal{B}(\Omega)$, and $\mathbb{I}_B$ stands for the indicator of B. We also set $\pi_\Lambda(\cdot|\xi) \equiv 0$ for $\xi \in \Omega \setminus \Omega^{\rm t}$. For every $\xi \in \Omega^{\rm t}$, $\pi_\Lambda(\cdot|\xi)$ is a probability measure on $(\Omega^{\rm t}, \mathcal{B}(\Omega^{\rm t}))$. The family $\{\pi_\Lambda\}_{\Lambda \Subset \mathbb{L}}$ is called the local Gibbs specification corresponding to the model (1).

DEFINITION 2.2. *A measure $\mu \in \mathcal{P}(\Omega)$ is called a (tempered) Euclidean Gibbs measure if it satisfies the Dobrushin-Lanford-Ruelle (equilibrium) equation*

$$\int_\Omega \pi_\Lambda(B|\omega)\mu(\mathrm{d}\omega) = \mu(B), \tag{36}$$

for all $\Lambda \Subset \mathbb{L}$ and $B \in \mathcal{B}(\Omega)$. The set of all such measures is denoted by $\mathcal{G}^{\rm t}$.

The elements of $\mathcal{G}^{\rm t}$ are supported by $\Omega^{\rm t}$, which follows from the corresponding property of π_Λ. By $\mathcal{W}^{\rm t}$ we denote the usual weak topology on the set of all probability measures $\mathcal{P}(\Omega^{\rm t})$.

3. The Results

3.1. The general case

THEOREM 3.1. *For every $\beta > 0$, the set $\mathcal{G}^{\rm t}$ is non-void and $\mathcal{W}^{\rm t}$-compact.*

Next we get an exponential moment estimate, similar to (18), in which the constant may depend on σ but is independent of $\mu \in \mathcal{G}^{\rm t}$ and $\ell \in \mathbb{L}$.

THEOREM 3.2. *For every $\sigma \in (0, 1/2)$, there exists $C > 0$ such that, for any $\ell \in \mathbb{L}$ and $\mu \in \mathcal{G}^{\rm t}$,*

$$\int_\Omega \exp\left(\lambda_\sigma |\omega_\ell|^2_{C^\sigma_\beta}\right) \mu(\mathrm{d}\omega) \leq C, \tag{37}$$

where λ_σ is the same as in (18).

The set of tempered configurations $\Omega^{\rm t}$, which is a supporting set for $\nu \in \mathcal{G}^{\rm t}$, was introduced in (33) by means of rather slack restrictions of L^2_β-norms of ω_ℓ. In fact, our Gibbs measures have a much smaller support (of Lebowitz-Presutti type), which is independent of the choice of the weights w_α. Given $b > 0$ and $\sigma \in (0, 1/2)$, we define

$$\Xi(b, \sigma) \ = \ \{\xi \in \Omega \mid (\forall \ell_0 \in \mathbb{L}) \ (\exists \Lambda_{\xi,\ell_0} \Subset \mathbb{L}) \ (\forall \ell \in \mathbb{L} \setminus \Lambda_{\xi,\ell_0}) : \\ |\xi_\ell|^2_{C^\sigma_\beta} \leq b \log(1 + |\ell - \ell_0|)\},$$

which is a Borel subset of $\Omega^{\rm t}$.

THEOREM 3.3. *For every $\sigma \in (0, 1/2)$, there exists $b > 0$, which depends on σ and on the parameters of the model only, such that*

$$\mu(\Xi(b, \sigma)) = 1, \quad \text{for all } \mu \in \mathcal{G}^{\rm t}. \tag{38}$$

The last result in this group gives a sufficient condition for $|\mathcal{G}^{\rm t}| = 1$, which holds at high temperatures. Let us decompose $V_\ell = V_{1,\ell} + V_{2,\ell}$, where $V_{1,\ell} \in C^2(\mathbb{R}^\nu)$, $V_{2,\ell}$ are such that

$$-a \leq b \ \stackrel{\rm def}{=} \ \inf_\ell \inf_{x,y \in \mathbb{R}^\nu, \ y \neq 0} (V''_{1,\ell}(x) y, y)/|y|^2 < +\infty, \tag{39}$$

$$0 \leq \delta \ \stackrel{\rm def}{=} \ \sup_\ell \left\{ \sup_{x \in \mathbb{R}} V_{2,\ell}(x) - \inf_{x \in \mathbb{R}} V_{2,\ell}(x) \right\} \leq +\infty.$$

The role of $V_{2,\ell}$ is to produce multiple wells responsible for eventual phase transitions.

THEOREM 3.4. *The set $\mathcal{G}^{\rm t}$ contains exactly one element if*

$$e^{\beta\delta} < (a + b)/\hat{J}_0. \tag{40}$$

The condition (40) is independent of the mass m, hence, the uniqueness stated holds also in the quasi-classical limit $m \to +\infty$ [3].

3.2. Scalar ferroelectric models

Here we consider the case $\nu = 1$, $J_{\ell\ell'} \geq 0$. For $\omega, \tilde{\omega} \in \Omega$, we set $\omega \leq \tilde{\omega}$ if for all ℓ and $\tau \in [0, \beta]$, one has $\omega_\ell(\tau) \leq \tilde{\omega}_\ell(\tau)$. A function $f : \Omega \to \mathbb{R}$ is called increasing if $\omega \leq \tilde{\omega}$ implies $f(\omega) \leq f(\tilde{\omega})$. For $\mu \in \mathcal{P}(\Omega^{\rm t})$ and a bounded continuous $f : \Omega^{\rm t} \to \mathbb{R}$, we write

$$\mu(f) = \int_{\Omega^{\rm t}} f(\omega) \mu({\rm d}\omega).$$

Then for $\mu_1, \mu_2 \in \mathcal{P}(\Omega^{\rm t})$, we set $\mu_1 \leq \mu_2$ if $\mu_1(f) \leq \mu_2(f)$ for all increasing f. One can show that this is an order on $\mathcal{P}(\Omega^{\rm t})$ (the FKG order).

THEOREM 3.5. *The set $\mathcal{G}^{\rm t}$ has a maximal μ_+ and a minimal μ_- elements. These elements are extreme; they are translation invariant if $\mathbb{L}$ is a lattice and the model is translation invariant. If $V_\ell(x) = V_\ell(-x)$ for all $\ell \in \mathbb{L}$, then $\mu_+(B) = \mu_-(-B)$ for all $B \in \mathcal{B}(\Omega)$.*

The next statement describes a phase transition in our model, which corresponds to $|\mathcal{G}^{\rm t}| > 1$. Here we suppose that $\mathbb{L} = \mathbb{Z}^d$ and

$$\inf_{\ell,\ell' :\ |\ell-\ell'|=1} J_{\ell\ell'} \ \stackrel{\rm def}{=}\ J > 0. \tag{41}$$

For $d \geq 3$, we set

$$\theta_d = \frac{1}{(2\pi)^d}\int_{(-\pi,\pi]^d} \frac{{\rm d}p}{E(p)}, \qquad E(p) = \sum_{j=1}^{d}[1 - \cos p_j]. \tag{42}$$

Let also $f : [0, +\infty) \to [0, 1)$ be the function defined implicitly by

$$f(t \tanh t) = t^{-1} \cdot \tanh t, \quad \text{for} \ \ t > 0, \ \ \text{and} \ \ f(0) = 1. \tag{43}$$

It is convex and monotone decreasing on $(0, +\infty)$. Furthermore, for every fixed $\alpha > 0$, the function

$$(0, +\infty) \ni t \mapsto \phi(t, \alpha) = \alpha t f(t/\alpha), \tag{44}$$

is monotone increasing to α^2 as $t \to +\infty$. Next we suppose that all V_ℓ are even continuous functions and the upper bound in (4) is

$$V(x_\ell) = \sum_{s=1}^{r} b^{(s)} x_\ell^{2s}; \quad 2b^{(1)} < -a; \quad b^{(s)} \geq 0, \ s \geq 2, \tag{45}$$

where a is as in (3) and $r \in \mathbb{N}$ or $r = +\infty$. In the latter case, the series

$$\sum_{s=2}^{r} \frac{(2s)!}{2^{s-1}(s-1)!} b^{(s)} t^{s-1} \ \stackrel{\rm def}{=}\ \Phi(t), \tag{46}$$

converges at some $t > 0$. In both cases the equation

$$2b^{(1)} + a + \Phi(t) = 0, \tag{47}$$

has a unique solution $t_* > 0$. Finally, we suppose that for every ℓ, $V(x_\ell) - V_\ell(x_\ell)$ is an increasing function of x_ℓ^2.

THEOREM 3.6. *Let $d \geq 3$ and the above assumptions hold. Then under the condition*

$$J > \theta_d / 8 m t_*^2, \tag{48}$$

there exists $\beta_* > 0$ such that $|\mathcal{G}^{\rm t}| > 1$ for $\beta > \beta_*$. The bound β_* is the unique solution of the equation

$$2\theta_d m / J = \phi(\beta, 4mt_*). \tag{49}$$

As is known [2, 5], quantum effects may stabilize quantum systems preventing them from any phase transition. The next result describes such effects for the model considered. Like above, all V_ℓ are supposed to be even continuous functions. In addition, we suppose that there exists a convex strictly increasing function $v : \mathbb{R}_+ \to \mathbb{R}$ such that for every ℓ, $V_\ell(x_\ell) - v(x_\ell^2)$ is an increasing function of x_ℓ^2. Then the Hamiltonian

$$\tilde{H}_\ell = -\frac{1}{2m}\left(\frac{\partial}{\partial x_\ell^{(j)}}\right)^2 + \frac{a}{2}x_\ell^2 + v(x_\ell^2),$$

has a discrete non-degenerate spectrum $\{E_n\}_{n\in\mathbb{N}}$. Set

$$\varDelta = \min_{n\in\mathbb{N}} \left(E_n - E_{n-1}\right). \tag{50}$$

THEOREM 3.7. *Under the above assumptions* $|\mathcal{G}^{\mathrm{t}}| = 1$ *if*

$$m\varDelta^2 > \hat{J}_0. \tag{51}$$

Note that (51) is a stability condition, in which $m\varDelta^2$ appears as the oscillator rigidity caused by quantum effects. If it holds, a stability-due-to-quantum-effects occurs [5]. If v is a polynomial of degree r, the quantum rigidity $m\varDelta^2$ is a continuous function of the particle mass m; it gets small as $m \to +\infty$. If $m \to 0+$, then $m\varDelta^2 = O(m^{-(r-1)/(r+1)})$; hence, (51) certainly holds in the small mass limit [2, 4, 5]. To compare this result with Theorem 3.6, suppose that $\mathbb{L} = \mathbb{Z}^d$, $J_{\ell\ell'} = J$ iff $|\ell - \ell'| = 1$, and all V_ℓ coincide with the function given by (45). Then the parameter (50) obeys the estimate $\varDelta < 1/2mt_*$, see [23], where t_* is the same as in (48). In this case (51) may be rewritten $J < 1/8dmt_*^2$. One can show that $\theta_d > 1/d$ and $d\theta_d \to 1$ as $d \to +\infty$; thus, the estimates (48) and (51) become precise in this limit.

Now let $\mathbb{L}$ be a lattice and the model (1) be translation invariant, i.e., $V = V_\ell$. We set

$$\mathcal{F} = \left\{\varphi : \mathbb{R} \to \mathbb{R} \;\middle|\; \varphi(t) = \varphi_0 \exp(\gamma_0 t) t^n \prod_{i=1}^{\infty}(1 + \gamma_i t)\right\}, \tag{52}$$

where $\varphi_0 > 0,\ n \in \mathbb{N}_0,\ \gamma_i \geq 0$ for all $i \in \mathbb{N}_0$, and $\sum_{i=1}^{\infty} \gamma_i < \infty$. Clearly, each $\varphi \in \mathcal{F}$ can be extended to an exponential type entire function $\varphi : \mathbb{C} \to \mathbb{C}$, which has no zeros outside of $(-\infty, 0]$. In the next theorem $a > 0$ is the same as in (3).

THEOREM 3.8. *Let the model be translation invariant and the anharmonicity potential* V *be of the form*

$$V(x) = v(x^2) - hx, \quad h \in \mathbb{R}, \tag{53}$$

where v is such that for a certain $b \geq a/2$, its derivative v' obeys the condition $b + v' \in \mathcal{F}$. Then $|\mathcal{G}^{\mathrm{t}}| = 1$ if $h \neq 0$.

3.3. Comments

We have given a rigorous description of the equilibrium thermodynamic properties of the quantum model (1) based on a path representation of local Gibbs states (9). In our approach, the model is represented by a system of infinite-dimensional spins; its global properties are described by the Gibbs measures constructed by means of the DLR approach. Since the spins are infinite-dimensional, our technique is more complicated than the one used for classical spins. Additional complications arise from the fact that we study a general case, where the model has no spacial regularity and the interaction is of infinite range. In view of the latter property, the only way to develop the theory is to impose a priori restrictions on the support of the Gibbs measures, which was done by means of the weights obeying the conditions (23) – (26). These conditions are competitive and, in principle, can contradict each other if the interaction decays too slowly. Once they are satisfied, the set of tempered Gibbs measures $\mathcal{G}^{\mathrm{t}}$ is non-void, Theorem 3.1. A posteriori, its elements have much smaller support than Ω^{t}, established by the conditions (23) – (26), which does not depend on the particular choice of the weights. If the interaction has finite range, the Gibbs measures can be defined with no support restrictions. However, in this case the set of all such measures may contain 'improper' elements, which have no physical meaning and hence should be excluded from the theory. This can be done by means of the weights obeying the same conditions, except for (26) which is obeyed automatically. Once this is done, the tempered Gibbs measures obtained have the support described by Theorem 3.3.

Now let us compare our results with those known for similar classical and quantum models. For non-quantum models of unbound spins, the existence of tempered Gibbs measures had been proven by means of the renowned Dobrushin criterion (Theorem 1 in [15]). The methods of its verification heavily employed the specific features of the models and could not be helpful in our study. Our proof, which is much simpler, is based on estimates like (37) obtained for the kernels (35). These estimates allowed us to prove the compactness of $\mathcal{G}^{\mathrm{t}}$ and the estimate (37) itself. Estimates like (37) can be proven in the so called analytic approach to the construction of $\mathcal{G}^{\mathrm{t}}$ [6, 7], which is alternative to the DLR approach. Our results improve the corresponding results of [6, 7] in the following: (a) the bound (37) is much stronger; (b) we excluded many technical restrictions on V_ℓ, e.g., differentiability. Furthermore, Theorem 3.4 is an improved version of the corresponding result of [8, 9]; Theorem 3.6 improves the result of [10]; Theorem 3.7 is an improved version of the result of [4]. Theorems 3.3, 3.5, and 3.8 are strongly improved and extended versions of the corresponding statements proven for non-quantum models in [11, 26]. Except for Theorems 3.6 and 3.8, our results can describe systems with spacial irregularities and/or with random components.

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