Equilibrium dynamics and phase transitions in quantum anharmonic crystals

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Abstract. For a system of interacting quantum anharmonic (double-welled) oscillators (quantum anharmonic crystal), it is shown that a phase transition can cause the equilibrium dynamics of a given oscillator to be reducible. This means that the oscillator prefers one of the wells. Sufficient conditions for this effect to occur at some temperature, or not to occur at all temperatures, are presented.

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INTRODUCTION

A one-dimensional anharmonic oscillator is described by the Hamiltonian

$$H = H^{\rm har} + V(q) = \frac{1}{2m}p^2 + \frac{a}{2}q^2 + V(q), \qquad a > 0, \tag{1}$$

where m is the particle mass, and p and q are the particle momentum and displacement, respectively. The anharmonic potential is supposed to be of the form

$$V(q) = \sum_{s=1}^{r} b_s q^{2s}, \qquad b_1 \in \mathbb{R}, \quad b_r > 0, \quad b_2, \ldots, b_{r-1} \geq 0, \quad r \geq 2. \tag{2}$$

For $b_1 < -a/2$, the potential energy in (1) has two symmetric wells. In the classical case, the Hamiltonian dynamics of the oscillator with such a potential energy is reducible. Here this means that in the low-energy states the particle is trapped in one of the wells, which can be detected by an observer. In the quantum case, the Hamiltonian (1) is a self-adjoint and lower bounded linear operator acting in the physical Hilbert space $\mathfrak{H} = L^2(\mathbb{R})$. Its spectrum consists entirely of simple eigenvalues E_n, $n \in \mathbb{N}_0$. Each of the corresponding normalized eigenfunctions ψ_n defines a state

$$\mathfrak{C} \ni A \mapsto \omega_n(A) = (\psi_n, A\psi_n)_{\mathfrak{H}}, \tag{3}$$

where $\mathfrak{C}$ is the algebra of all bounded linear operators $A : \mathfrak{H} \to \mathfrak{H}$. The elements of $\mathfrak{C}$ are often called *observables*. The (Heisenberg) dynamics of the oscillator is described by the family $\{\mathfrak{a}^t\}_{t\in\mathbb{R}}$ of maps $\mathfrak{a}^t : \mathfrak{C} \to \mathfrak{C}$, where $t = \text{time}/\hbar^2$ and

$$\mathfrak{a}^t(A) = \exp(\mathrm{i}tH)A\exp(-\mathrm{i}tH). \tag{4}$$

As $\mathfrak{a}^t \circ \mathfrak{a}^s = \mathfrak{a}^{t+s}$, that is, $\mathfrak{a}^t(\mathfrak{a}^s(A)) = \mathfrak{a}^{t+s}(A)$, the family $\{\mathfrak{a}^t\}_{t\in\mathbb{R}}$ is a group. Clearly, each state ω_n is pure and hence ergodic, which means that $\omega_n \circ \mathfrak{a}^t = \omega_n$ and the restriction of the family $\exp(\mathrm{i}tH)$, $t \in \mathbb{R}$, to the subspace spanned by ψ_n is irreducible, see e.g. page 47 in [15]. This also means that the measurement in the computational basis $\{\psi_n\}_{n\in\mathbb{N}_0}$ cannot indicate which well is preferred by the oscillator.

Suppose now that our quantum oscillator interacts with an infinite number of its copies, which constitute a crystal lattice, say $\mathbb{Z}^\nu$. Suppose also that the whole system is in thermal equilibrium. The aim of the present note is to show that a phase transition in the infinite system can cause a reducibility of the oscillator dynamics, which, in particular, means that it prefers one of the wells.

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EQUILIBRIUM STATES

The model

As was already mentioned, we study an infinite system of interacting quantum oscillators (1), indexed by the vertices of the lattice $\mathbb{Z}^\nu$, $\nu \in \mathbb{N}$. This system is described by the formal Hamiltonian

$$\mathscr{H} = -\frac{1}{2}\sum_{\ell,\ell'} J_{\ell\ell'} q_\ell q_{\ell'} + \sum_\ell H_\ell, \tag{5}$$

in which p_ℓ and q_ℓ are the momentum and displacement operators of the oscillator located at $\ell \in \mathbb{Z}^\nu$, and H_ℓ is a copy of (1) with p and q replaced by p_ℓ and q_ℓ, respectively. The interaction intensities $J_{\ell\ell'}$ are supposed to be translation invariant and such that

$$\text{(i)} \quad J_{\ell\ell'} \geq 0, \qquad\qquad \text{(ii)} \quad \hat{J} \stackrel{\text{def}}{=} \sum_{\ell'} J_{\ell\ell'} < \infty. \tag{6}$$

The model defined by the Hamiltonian (5) is called *a quantum anharmonic crystal*. If in (5) one takes H_ℓ^{har} instead of H_ℓ, the corresponding model is called *a quantum harmonic crystal*. The latter is *stable* if

$$\hat{J} < a. \tag{7}$$

By writing $\Lambda \Subset \mathbb{Z}^\nu$ we mean that Λ is a non-void and finite set of vertices. A sequence $\mathscr{L}$ of such sets is said to be *cofinal* if it is ordered by inclusion and exhausts the lattice, that is, each ℓ belongs to a certain $\Lambda \in \mathscr{L}$. The Hamiltonian (5) has no direct mathematical meaning and is usually 'represented' by its *local* versions

$$H_\Lambda = -\frac{1}{2}\sum_{\ell,\ell' \in \Lambda} J_{\ell\ell'} q_\ell q_{\ell'} + \sum_{\ell \in \Lambda} H_\ell, \qquad \Lambda \Subset \mathbb{Z}^d. \tag{8}$$

In the sequel, a property related with a set $\Lambda \Subset \mathbb{Z}^\nu$ will be called local, whereas *global* will always refer to a property of the whole infinity model. Each local Hamiltonian H_Λ is a self-adjoint lower bounded operator in $\mathfrak{H}_\Lambda = L^2(\mathbb{R}^{|\Lambda|})$, such that for any $\beta > 0$,

$$Z_\Lambda \stackrel{\text{def}}{=} \text{trace} \exp\left(-\beta H_\Lambda\right) < \infty. \tag{9}$$

Along with (8) one can also consider the harmonic local Hamiltonians H_Λ^{har}. However, the latter operators are lower bounded for all $\Lambda \Subset \mathbb{Z}^\nu$ only if the stability condition (7) is satisfied.

Local states and local Euclidean Gibbs measures

Given $\Lambda \Subset \mathbb{Z}^\nu$, the portion of oscillators located in Λ is described by the Hamiltonian H_Λ, which has a discrete spectrum consisting entirely of eigenvalues of finite multiplicity $E_\Lambda^{(n)}$, $n \in \mathbb{N}$. The corresponding normalized eigenfunctions $\psi_\Lambda^{(n)}$ constitute a basis of the physical Hilbert space $\mathfrak{H}_\Lambda$. As in the case of a single oscillator, the eigenfunctions define pure states

$$\mathfrak{C}_\Lambda \ni A \mapsto \omega_\Lambda^{(n)}(A) = (\psi_\Lambda^{(n)}, A\psi_\Lambda^{(n)})_{\mathfrak{H}_\Lambda}, \tag{10}$$

whereas the dynamics of the observables is defined by the maps $\mathfrak{a}_\Lambda^t : \mathfrak{C}_\Lambda \to \mathfrak{C}_\Lambda$, $t \in \mathbb{R}$,

$$\mathfrak{a}_\Lambda^t(A) = \exp\left(\mathrm{i}H_\Lambda t\right) A \exp\left(-\mathrm{i}H_\Lambda t\right). \tag{11}$$

Here and in (10), $\mathfrak{C}_\Lambda$ stands for the algebra of all bounded linear operators $A : \mathfrak{H}_\Lambda \to \mathfrak{H}_\Lambda$. The group $\{\mathfrak{a}_\Lambda^t\}_{t\in\mathbb{R}}$ describes the (reversible) dynamics of the considered portion of oscillators. We note, however, that this description ignores the existence and hence the effect of the oscillators located outside Λ.

Along with the states $\omega_\Lambda^{(n)}$, $n \in \mathbb{N}_0$, one can consider their convex combination with the coefficients proportional to $\exp(-\beta E_\Lambda^{(n)})$ for some $\beta > 0$. That is, such a state is

$$\mathfrak{C}_\Lambda \ni A \mapsto \gamma_\Lambda(A) = \sum_{n=0}^{\infty} \omega_\Lambda^{(n)}(A) \exp\left(-\beta E_\Lambda^{(n)}\right) / Z_\Lambda,$$

where Z_Λ is as in (9). It can be viewed as the state of thermal equilibrium of the considered portion of oscillators at temperature $T = 1/k_{\rm B}\beta$. Obviously,

$$\gamma_\Lambda(A) = \mathrm{trace}(AR_\Lambda), \qquad R_\Lambda = \exp\left(-\beta H_\Lambda\right)/Z_\Lambda. \tag{12}$$

The state γ_Λ has a property, which reflects a consistency of the thermodynamic behavior of the considered system with its dynamics described by the maps (11). This property is usually referred to as the KMS property relative to the group $\{\mathfrak{a}^t_\Lambda\}_{t\in\mathbb{R}}$, see [3, 5, 7]. According to it, for each $A,B \in \mathfrak{C}_\Lambda$, there exists a function $f_{A,B}(z)$, analytic in the open strip $\{z \in \mathbb{C} \mid 0 < \mathrm{Im} z < \beta\}$ and continuous on its closure, such that for all $t \in \mathbb{R}$,

$$f_{A,B}(t) = \gamma_\Lambda(A\mathfrak{a}^t_\Lambda(B)), \qquad f_{A,B}(t+\mathrm{i}\beta) = \gamma_\Lambda(\mathfrak{a}^t_\Lambda(B)A). \tag{13}$$

One can show that for a fixed β, γ_Λ is the only KMS state on $\mathfrak{C}_\Lambda$.

Given $F \in L^\infty(\mathbb{R}^{|\Lambda|})$, the multiplication operator, which we also denote by F, acts in $\mathfrak{H}_\Lambda$ as

$$(F\phi)(x) = F(x)\phi(x).$$

Clearly, $F \in \mathfrak{C}_\Lambda$. Let $\mathfrak{M}_\Lambda$ be the set of all such multiplication operators. It is a maximal abelian $*$-sub-algebra[1] of $\mathfrak{C}_\Lambda$. One can prove, see [12] or [2], Theorem 1.2.24 on page 72, that the linear span of the operators

$$\mathfrak{a}^{t_1}_\Lambda(F_1)\cdots\mathfrak{a}^{t_n}_\Lambda(F_n) \tag{14}$$

with all possible choices of $n \in \mathbb{N}$, $t_1,\ldots,t_n \in \mathbb{R}$, and $F_1,\ldots,F_n \in \mathfrak{M}_\Lambda$, is σ-weakly dense in the algebra $\mathfrak{C}_\Lambda$. At the same time, the state γ_Λ is normal and hence σ-weakly continuous, see [4], page 65. Thus, γ_Λ is fully determined by its values on the products (14), that is, by *the Green functions*

$$G^\Lambda_{F_1,\ldots,F_n}(t_1,\ldots,t_n) = \gamma_\Lambda\left(\mathfrak{a}^{t_1}_\Lambda(F_1)\cdots\mathfrak{a}^{t_n}_\Lambda(F_n)\right). \tag{15}$$

The state γ_Λ and the maps (11) can be extended to certain unbounded operators, among which we distinguish displacement operators q_ℓ, $\ell \in \Lambda$, cf. Proposition 1.2.14 in [2], page 70. Thus, we can also define the following Green functions

$$G^\Lambda_{\ell_1,\ldots,\ell_n}(t_1,\ldots,t_n) = \gamma_\Lambda\left(\mathfrak{a}^{t_1}_\Lambda(q_{\ell_1})\cdots\mathfrak{a}^{t_n}_\Lambda(q_{\ell_n})\right). \tag{16}$$

It turns out that the linear span of the products (14) is σ-weakly dense in $\mathfrak{C}_\Lambda$ if one takes F_i's from sets of multiplication operators smaller than the whole $\mathfrak{M}_\Lambda$.

Definition 1: A set of operators $\mathfrak{F} \subset \mathfrak{M}_\Lambda$ is said to be a complete family if the set of operators (14) with all possible choices of $n \in \mathbb{N}$, $t_1,\ldots,t_n \in \mathbb{R}$, and $F_1,\ldots,F_n \in \mathfrak{F}$, is σ-weakly dense in $\mathfrak{C}_\Lambda$. This is equivalent to the property that if ω is a state on $\mathfrak{C}_\Lambda$ such that for all $n \in \mathbb{N}$, $t_1,\ldots,t_n \in \mathbb{R}$, and $F_1,\ldots,F_n \in \mathfrak{F}$,

$$\omega\left\{\mathfrak{a}^{t_1}_\Lambda(F_1)\cdots\mathfrak{a}^{t_n}_\Lambda(F_n)\right\} = G^\Lambda_{F_1,\ldots,F_n}(t_1,\ldots,t_n),$$

then $\omega = \gamma_\Lambda$.

It is known, see Theorem 1.3.26 on page 113 in [2] as well as Lemma 2.6 in [13], that if $\mathfrak{F}$ is a family of multiplication operators by continuous functions which is closed under multiplication, contains the identity operator, and separates points, then it is complete. The latter property means that for every distinct $x,y \in \mathbb{R}^{|\Lambda|}$, one finds $F \in \mathfrak{F}$ such that the corresponding function takes distinct values on these x and y. By means of this fact we can prove the following statement.

Proposition 1: *Let $\mathfrak{Q}_\Lambda$ be the family of multiplication operators by the functions*

$$Q_\lambda(x) = \exp\left(\mathrm{i}\sum_{\ell\in\Lambda}\lambda_\ell x_\ell\right), \tag{17}$$

with all possible choices of rational λ_ℓ, $\ell \in \Lambda$. Then $\mathfrak{Q}_\Lambda$ is complete.

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[1] $\mathfrak{M}_\Lambda$ is a von Neumann algebra.

It is known, see Theorem 1.2.32, page 78 in [2] or Theorem 2.1 in [7], that the Green functions (15) can be considered as restrictions of functions, which we denote by $G^{\Lambda}_{F_1,\ldots,F_n}(z_1,\ldots,z_n)$, analytic in the domain

$$\mathscr{D}^n_\beta = \{(z_1,\ldots,z_n)\in\mathbb{C}^n \mid 0<\mathrm{Im}z_1<\mathrm{Im}z_2<\cdots<\mathrm{Im}z_n<\beta\}, \tag{18}$$

and continuous on its closure $\overline{\mathscr{D}^n_\beta}$. Moreover, for every $n\in\mathbb{N}$, the 'imaginary time' subset

$$\mathscr{D}^n_\beta(0) = \{(z_1,\ldots,z_n)\in\mathscr{D}^n_\beta \mid \mathrm{Re}z_1=\cdots=\mathrm{Re}z_n=0\}$$

is a set of uniqueness for functions analytic in $\mathscr{D}^n_\beta$, which means that such two functions coincide if they coincide on $\mathscr{D}^n_\beta(0)$. This fact is known as *the multiple-time analyticity*, cf. Section 2 in [7]. Therefore, the Green functions (15), and hence the state γ_Λ, are completely determined by *the Matsubara* (another name *thermal Green*) functions

$$\begin{aligned}\Gamma^{\Lambda}_{F_1,\ldots,F_n}(\tau_1,\ldots,\tau_n) &= G^{\Lambda}_{F_1,\ldots,F_n}(\mathrm{i}\tau_1,\ldots,\mathrm{i}\tau_n) \\ &= \mathrm{trace}\left[F_1 e^{-(\tau_2-\tau_1)H_\Lambda}\cdot F_2 e^{-(\tau_3-\tau_2)H_\Lambda}\cdots F_n e^{-(\tau_{n+1}-\tau_n)H_\Lambda}\right]/Z_\Lambda,\end{aligned} \tag{19}$$

with $0\le\tau_1\le\cdots\le\tau_n\le\tau_1+\beta \stackrel{\mathrm{def}}{=} \tau_{n+1}$ and all possible choices of $F_1,\ldots,F_n$ in a complete family. The central element of the Euclidean approach[2] is the representation of the Matsubara functions (19) in the form

$$\Gamma^{\Lambda}_{F_1,\ldots,F_n}(\tau_1,\ldots,\tau_n) = \int_{\Xi_\Lambda} F_1(\xi(\tau_1))\cdots F_n(\xi(\tau_n))\mu_\Lambda(\mathrm{d}\xi), \tag{20}$$

where μ_Λ is a certain probability measure on the space Ξ_Λ of paths $\xi=(\xi_\ell)_{\ell\in\Lambda}$, each ξ_ℓ being a continuous function $\xi_\ell:[0,\beta]\to\mathbb{R}$, such that $\xi_\ell(0)=\xi_\ell(\beta)$. By standard arguments, the measure μ_Λ is uniquely determined by the integrals (20). Since the Matsubara functions uniquely determine the state γ_Λ, the representation (20) establishes a one-to-one correspondence between the local Gibbs states γ_Λ and the measures μ_Λ, called *local Euclidean Gibbs measures.*

Let $\mathfrak{M}^+_\Lambda$ be the set of multiplication operators by functions, which take real nonnegative values only. The representation (20) immediately yields that for $F_1,\ldots,F_n\in\mathfrak{M}^+_\Lambda$, one has

$$\Gamma^{\Lambda}_{F_1,\ldots,F_n}(\tau_1,\ldots,\tau_n)\ge 0 \tag{21}$$

for all $\tau_1,\ldots,\tau_n$. Furthermore, if $\Gamma^{\Lambda}_{F_1,\ldots,F_n}$ is identically zero, then all F_i, $i=1,\ldots,n$, are equal to the zero operator. This property can also be obtained from the fact that γ_Λ is a faithful state, that is, $\gamma_\Lambda(A)=0$ implies that A is the zero operator. Summing up all these facts we conclude that the tuple $(\mathfrak{C}_\Lambda,\mathfrak{M}_\Lambda,\{\mathfrak{a}^t_\Lambda\}_{t\in\mathbb{R}},\gamma_\Lambda)$ is *a stochastically positive KMS system*, cf. Definition 3.2 in [7].

Global states of thermal equilibrium

In the Euclidean approach which we follow in this note, the description of thermodynamic phases of the model (5) existing at a given β is made by constructing the set of *tempered Euclidean Gibbs measures* $\mathscr{G}^{\mathrm{t}}_\beta$, see [2, 9, 14]. By definition, each $\mu\in\mathscr{G}^{\mathrm{t}}_\beta$ is a probability measure on *the space of tempered configurations* Ξ^{t}, which solves the so-called equilibrium (another name *Dobrushin-Lanford-Ruelle*) equation[3], formulated with the aid of the Hamiltonians (8). It can be shown, see Theorem 3.1 in [14] and Theorem 3.3.6, page 216 of [2], that for the model (5) the set $\mathscr{G}^{\mathrm{t}}_\beta$ is non-void. Furthermore, as the equilibrium equation is linear, for any μ_1 and μ_2 which solve this equation, the measure $\mu=\theta\omega_1+(1-\theta)\omega_2$, $\theta\in[0,1]$, also solves it. Therefore, the set $\mathscr{G}^{\mathrm{t}}_\beta$ is convex. An element $\mu\in\mathscr{G}^{\mathrm{t}}_\beta$ is said to be *extreme* if the fact that $\mu=\theta\mu_1+(1-\theta)\mu_2$ for some $\mu_1,\mu_2\in\mathscr{G}^{\mathrm{t}}_\beta$ and $\theta\in[0,1]$, implies that $\mu=\mu_1$ or $\mu=\mu_2$. Clearly, if $\mathscr{G}^{\mathrm{t}}_\beta$ is a singleton, its only element is extreme. Extreme elements of $\mathscr{G}^{\mathrm{t}}_\beta$, possessing an additional property,

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[2] A complete exposition of this approach can be found in [2], see also [14].

[3] See Chapter 2 of [6] for more details.

correspond to equilibrium phases of the model (5) in the following sense[4]. Take any $F \in \mathfrak{M}_{\Lambda_0}$ for some $\Lambda_0 \Subset \mathbb{Z}^d$. Then this F can also be considered as an element of every $\mathfrak{M}_\Lambda$ such that Λ_0 is contained in Λ. The corresponding function F just depends on fewer variables. In view of this, we define

$$\mathfrak{M} = \bigcup_{\Lambda \Subset \mathbb{Z}^\nu} \mathfrak{M}_\Lambda,$$

and call $\mathfrak{M}$ *the set of all local multiplication operators*. For any $F_1, \ldots, F_n \in \mathfrak{M}$, $\tau_1, \ldots, \tau_n \in [0, \beta]$, and $\mu \in \mathscr{G}^{\mathrm{t}}_\beta$, the integrals, cf. (20),

$$\Gamma^\mu_{F_1,\ldots,F_n}(\tau_1, \ldots, \tau_n) \stackrel{\mathrm{def}}{=} \int_{\Xi^{\mathrm{t}}} F_1(x(\tau_1)) \cdots F_n(x(\tau_n))\mu(\mathrm{d}x), \tag{22}$$

are called Matsubara functions corresponding to this μ. We say that μ is *τ-shift invariant* if

$$\Gamma^\mu_{F_1,\ldots,F_n}(\tau_1 + \vartheta, \ldots, \tau_n + \vartheta) = \Gamma^\mu_{F_1,\ldots,F_n}(\tau_1, \ldots, \tau_n), \tag{23}$$

for any $F_1, \ldots, F_n \in \mathfrak{M}$ and any $\vartheta \in [0, \beta]$, where the addition $\tau_i + \vartheta$, $i = 1, \ldots, n$, is of modulo β. Let $\mathscr{G}^{\mathrm{phase}}_\beta$ be the subset of $\mathscr{G}^{\mathrm{t}}_\beta$ consisting of extreme and τ-shift invariant measures. Then each $\mu \in \mathscr{G}^{\mathrm{phase}}_\beta$ is said to be a state of thermal equilibrium of the quantum crystal described by the Hamiltonian (5). It is defined by its Matsubara functions (22) corresponding to all possible choices of $n \in \mathbb{N}$ and local multiplication operators $F_1, \ldots, F_n \in \mathfrak{M}$. Such states are also called equilibrium phases, existing at a given value of β. As was noted above, our model (5) has at least one such phase for any $\beta > 0$. If for a given β, the set $\mathscr{G}^{\mathrm{t}}_\beta$ consists of a single element, this element is automatically extreme and τ-shift invariant. Hence, in this case there exists only one equilibrium phase. As is commonly accepted, see [6], phase transitions are associated with the existence of multiple equilibrium phases at the same temperature. Thus, we say that the model (5) has a phase transition if the set $\mathscr{G}^{\mathrm{phase}}_\beta$ contains more than one element for some $\beta > 0$. In this case, the model has also a first-order phase transition in the sense of L. D. Landau, see Theorem 6.1.9, page 289 in [2], or Theorem 3.3 in [8].

For a given $\ell_0 \in \mathbb{Z}^\nu$ and $x = (x_\ell)_{\ell \in \mathbb{Z}^\nu}$, we set $s_{\ell_0}(x) = (x_{\ell+\ell_0})_{\ell \in \mathbb{Z}^\nu}$; that is, s_{ℓ_0} is a spatial shift. Then, for the same ℓ_0 and $F \in \mathfrak{M}$, the 'shifted' operator $\sigma_{\ell_0}(F)$ is set to be the multiplication operator by the function

$$\sigma_{\ell_0}(F)(x) = F\left(s_{\ell_0}(x)\right).$$

Clearly, $\sigma_{\ell_0}(F) \in \mathfrak{M}$ for any ℓ_0. A given $\mu \in \mathscr{G}^{\mathrm{phase}}_\beta$ is said to be *translation invariant* if for every $\ell_0 \in \mathbb{Z}^\nu$,

$$\Gamma^\mu_{F_1,\ldots,F_n} = \Gamma^\mu_{\sigma_{\ell_0}(F_1),\ldots,\sigma_{\ell_0}(F_n)}, \tag{24}$$

for all choices of $n \in \mathbb{N}$ and $F_1, \ldots, F_n \in \mathfrak{M}$. With this regard, we note that elements of the set $\mathscr{G}^{\mathrm{phase}}_\beta$ need not be translation invariant. However, if $\mathscr{G}^{\mathrm{phase}}_\beta$ is a singleton, its unique element is translation invariant, which follows from the translation invariance of the model (5).

With the aid of Theorem 3.3.1, page 214 in [2], see also Theorem 3.2 in [14], one can show that for every $\mu \in \mathscr{G}^{\mathrm{phase}}_\beta$, cf. (19),

$$M^\mu_\ell \stackrel{\mathrm{def}}{=} \int_{\Xi^{\mathrm{t}}} \xi_\ell(\tau)\mu(\mathrm{d}\xi) < \infty. \tag{25}$$

By (23), M^μ_ℓ is independent of τ; it is also independent of ℓ if μ is translation invariant. In the latter case, we say that M^μ is *the spontaneous polarization*[5] in state μ.

It can be shown, see Theorem 3.7.4, page 240 in [2], or Theorem 3.8 in [14], that the set $\mathscr{G}^{\mathrm{phase}}_\beta$ contains two translation invariant elements, $\mu^\pm$, such that for any ℓ and $\mu \in \mathscr{G}^{\mathrm{phase}}_\beta$,

$$M^{\mu^-} \leq M^\mu_\ell \leq M^{\mu^+}, \qquad M^{\mu^-} = -M^{\mu^+}. \tag{26}$$

[4] See Chapter 7 of [6].

[5] We employ here a 'ferroelectric' terminology – in a 'ferromagnetic' one, M^μ is a magnetization.

Furthermore, $\mathscr{G}_\beta^{\text{phase}}$ is a singleton if and only if $M^{\mu^-} = M^{\mu^+} = 0$. The measures $\mu^\pm$, and hence their Matsubara functions, can be obtained in a certain way, which sheds additional light on their properties. For a certain $y^\pm = (y_\ell^\pm)_{\ell\in\mathbb{Z}^\nu}, y_\ell^\pm \in \mathbb{R}$, and $\Lambda \Subset \mathbb{Z}^\nu$, we set, see (8),

$$H_\Lambda^\pm = H_\Lambda - \sum_{\ell\in\Lambda} y_\ell^\pm q_\ell. \tag{27}$$

Let $\gamma_\Lambda^\pm$ be the states defined according to (12) with H_Λ replaced by $H_\Lambda^\pm$. For these states, we define the Green functions (15) and hence the Matsubara functions (19), which we denote by $\Gamma_{F_1,\dots,F_n}^{\Lambda,\pm}$. It can be proven, see Section 7.2 in [14], that for any cofinal sequence $\mathscr{L}$, one can choose sequences $\{y_\Lambda^\pm\}_{\Lambda\in\mathscr{L}}$ in such a way that for any $F_1,\dots,F_n \in \mathfrak{M}$,

$$\lim_{\Lambda\in\mathscr{L}} \Gamma_{F_1,\dots,F_n}^{\Lambda,\pm} = \Gamma_{F_1,\dots,F_n}^{\mu^\pm}, \tag{28}$$

where the convergence is such that the functions $\Gamma_{F_1,\dots,F_n}^{\mu^\pm}$ can be continued to functions $G_{F_1,\dots,F_n}^{\mu^\pm}(z_1,\dots,z_n)$, analytic in the domain (18). By (28), and (15) and (11) we easily get the following two properties of $\Gamma_{F_1,\dots,F_n}^{\mu^\pm}$:

(i) for any $j = 1,\dots n-1$,

$$\Gamma_{F_1,\dots,F_{j-1},F_j,F_{j+1},F_{j+2},\dots,F_n}^{\mu^\pm}(\tau_1,\dots,\tau_{j-1},\tau_j,\tau_j,\tau_{j+2},\dots,\tau_n) \tag{29}$$

$$= \Gamma_{F_1,\dots,F_{j-1},F_{j,j+1},F_{j+2},\dots,F_n}^{\mu^\pm}(\tau_1,\dots,\tau_{j-1},\tau_j,\tau_{j+2},\dots,\tau_n),$$

where $F_{j,j+1} = F_j \cdot F_{j+1}$;

(ii) for any $j = 1,\dots n$, if F_j is the identity operator, then

$$\Gamma_{F_1,\dots,F_{j-1},F_j,F_{j+1},\dots,F_n}^{\mu^\pm}(\tau_1,\dots,\tau_{j-1},\tau_j,\tau_j,\dots,\tau_n) \tag{30}$$

$$= \Gamma_{F_1,\dots,F_{j-1},F_{j+1},\dots,F_n}^{\mu^\pm}(\tau_1,\dots,\tau_{j-1},\tau_{j+1},\dots,\tau_n).$$

THE RESULTS

In this section, we show that the dynamics of the portion of oscillators in a given $\Lambda \Subset \mathbb{Z}^d$, which are in thermal equilibrium with the rest of the crystal, can be reducible. This naturally includes the case of a single oscillator, i.e., the case of $\Lambda = \{\ell\}$. The dynamics of such a portion is described in the following way. For a C^*-algebra of multiplication operators $\mathfrak{N} \subset \mathfrak{M}_\Lambda$, which is σ-weakly dense in $\mathfrak{M}_\Lambda$, we construct a stochastically positive KMS system $(\mathfrak{A}, \mathfrak{B}, \{\mathfrak{a}^t\}_{t\in\mathbb{R}}, \omega)$ and define an injective homomorphism $\pi : \mathfrak{N} \to \mathfrak{B}$ such that for any $n \in \mathbb{N}, F_1,\dots,F_n \in \mathfrak{N}$, the Matsubara function $\Gamma_{\pi(F_1),\dots,\pi(F_n)}^{\omega}$, obtained by the multiple-time analyticity, cf. (19), from the Green function

$$G_{\pi(F_1),\dots,\pi(F_n)}^{\omega}(t_1,\dots,t_n) = \omega\left\{\mathfrak{a}^{t_1}(\pi(F_1))\cdots\mathfrak{a}^{t_n}(\pi(F_n))\right\} \tag{31}$$

satisfies the condition

$$\Gamma_{\pi(F_1),\dots,\pi(F_n)}^{\omega} = \Gamma_{F_1,\dots,F_n}^{\mu}, \tag{32}$$

for some $\mu \in \mathscr{G}_\beta^{\text{phase}}$. The precise formulation of this result is given in the next statement.

Theorem: *Let $\mathfrak{N}$ be the norm closure of the linear span of the family $\mathfrak{Q}_\Lambda$ defined in Proposition 1. Then for both of $\mu^\pm \in \mathscr{G}_\beta^{\text{phase}}$, there exists a stochastically positive KMS system $(\mathfrak{A}_\pm, \mathfrak{B}_\pm, \{\mathfrak{a}_\pm^t\}_{t\in\mathbb{R}}, \omega_\pm)$ and an injective homomorphism $\pi : \mathfrak{N} \to \mathfrak{B}_\pm$, such that (32) holds for all $n \in \mathbb{N}$ and $F_1,\dots,F_n \in \mathfrak{N}$.*

The proof of this statement readily follows from Theorem 3.1 of [3] by the properties (29) and (30), and by the fact that the linear span of $\mathfrak{Q}_\Lambda$ is countable and hence $\mathfrak{N}$ is a separable Banach space. The meaning of this mathematical result can be interpreted as follows. By (31) and (32) the Matsubara functions $\Gamma_{F_1,\dots,F_n}^{\mu^\pm}$ of the phases $\mu^\pm$ can be analytically continued to real time. This yields the corresponding Green functions $G^{\mu^\pm}_{F_1,\ldots,F_n}$, which, as we know, completely determine the dynamics of the system in the corresponding equilibrium state. This also relates to the functions (16). In particular, one can get the two-point correlation functions $G^{\mu^\pm}_{q_\ell,q_{\ell'}}(t,t')$. Then if the states μ^+ and μ^- are distinct, these functions are also distinct. Since

$$G^{\mu^+}_{q_\ell,q_{\ell'}}(t,t') = G^{\mu^-}_{-q_\ell,-q_{\ell'}}(t,t'),$$

the oscillators in Λ distinguish between the wells in this case, which can be experimentally detected. Of course, the reducibility can also be observed by measuring the spontaneous polarization, see (26).

The rest of the note will be devoted to presenting sufficient conditions for $\mu^+ \neq \mu^-$ for some β, or for $\mu^+ = \mu^-$ for all β.

Set

$$\mathscr{E}(k) = \sum_{j=1}^{\nu}[1-\cos k_j], \qquad k=(k_1,\ldots,k_\nu)\in(-\pi,\pi]^\nu, \tag{33}$$

and

$$\mathscr{I}(\nu) = \frac{\nu}{(2\pi)^\nu}\int_{(-\pi,\pi]^\nu}\frac{\mathrm{d}k}{\mathscr{E}(k)}. \tag{34}$$

Note that the latter integral is finite whenever $\nu \geq 3$. One can show, see e.g. Proposition 3.7 in [8], that for $\nu \geq 4$,

$$\frac{\nu}{\nu-1/2} < \mathscr{I}(\nu) < \frac{\nu}{\nu-1}. \tag{35}$$

In the formulation of our results, we employ the function $f:[0,+\infty)\to[0,1)$ defined implicitly by

$$f(u\tanh u) = u^{-1}\tanh u, \qquad f(0)=0.$$

This function is differentiable, convex, and monotonously decreasing to zero, such that $uf(u)\to 1$. For $u\geq 6$, $f(u)\approx 1/u$ to five-place accuracy. For $\alpha>0$, we set

$$\varphi(u) = u\alpha f(u/\alpha), \qquad u>0. \tag{36}$$

By computing φ' from the definition of f, one shows that φ is monotonously increasing to α^2 as $u\to+\infty$. For $b_2,\ldots,b_r$, the same as in (2), we set

$$\Phi(t) = \sum_{s=2}^{r}\frac{(2s)!}{2^{s-1}(s-1)!}b_s t^{s-1}, \qquad t\geq 0. \tag{37}$$

Suppose that $b_1 < -a/2$, that is the potential energy of the oscillator (1) has two wells. Then the equation

$$a + 2b_1 + \Phi(t) = 0 \tag{38}$$

has a unique positive solution t_*. Suppose that the interaction intensities $J_{\ell\ell'}$ in (5) are positive for $|\ell-\ell'|=1$. Thus, $J \stackrel{\text{def}}{=} J_{\ell\ell'}>0$ for such ℓ,ℓ'. The next statement was proven in [8] as Theorem 3.1, see also Theorem 6.3.8, page 310 in [2].

Proposition 2: *Let $\nu\geq 3$ and the following condition be satisfied*

$$8mt_*^2\nu J > \mathscr{I}(\nu), \tag{39}$$

where m is the particle mass. Then $\mu^+\neq\mu^-$ for every $\beta>\beta_*$, where the latter is the unique solution of the equation

$$2\nu J\beta f(\beta/4mt_*) = \mathscr{I}(\nu),$$

and f is as in (36).

As was mentioned above, the spectrum of the Hamiltonian (1) consists entirely of simple eigenvalues E_n, $n\in\mathbb{N}_0$. Thus, the following parameter

$$\Delta = \min_{n\in\mathbb{N}}(E_n - E_{n-1}) \tag{40}$$

is positive. It can be shown, see [11] or Theorem 1.1.60, page 59 in [2], that Δ is a continuous function of m, such that $\Delta \sim \Delta_0 m^{-r/(r+1)}$, as $m \to 0$, where r is the same as in (2). Therefore, $\mathfrak{r} \stackrel{\text{def}}{=} m\Delta^2$ is also a continuous function of m, such that $\mathfrak{r} \sim \Delta_0^2 m^{-(r-1)/(r+1)}$ as $m \to 0$. In the harmonic case, $\mathfrak{r} = a$; thereby, in the anharmonic case it can be called *a quantum rigidity* of the oscillator. The next statement (as Theorem 3.13) was proven in [14], see also Theorem 7.3.1, page 346 in [2].

Proposition 3: *The set of Euclidean Gibbs measures $\mathscr{G}_\beta^{\mathrm{t}}$ consists of exactly one element if the following stability condition is satisfied, cf. (7),*

$$m\Delta^2 > \hat{J}. \tag{41}$$

Note that the above result is independent of β. As $r \geq 2$, see (2), the condition (41) always holds for sufficiently small m. In [1], see also [10], such an effect was called *quantum stabilization.* It can be shown, see [11], that $\Delta < 1/2mt_*$, where t_* is the same as in Proposition 2. If $J_{\ell\ell'} = J$ for $|\ell - \ell'| = 1$, and $J_{\ell\ell'} = 0$ for $|\ell - \ell'| > 1$, then the condition (41) implies

$$8mt_*^2 \nu J < 1,$$

which can be compared with (39), see (35).

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