Phase transitions and quantum effects in anharmonic crystals

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(Dated: December 8, 2011)

The most important recent results in the theory of phase transitions and quantum effects in quantum anharmonic crystals are presented and discussed. In particular, necessary and sufficient conditions for a phase transition to occur at some temperature are given in the form of simple inequalities involving the interaction strength and the parameters describing a single oscillator. The main characteristic feature of the theory is that both mentioned phenomena are described in one and the same setting, in which thermodynamic phases of the model appear as probability measures on path spaces. Then the possibility of a phase transition to occur is related to the existence of multiple phases at the same values of the relevant parameters. Other definitions of phase transitions, based on the non-differentiability of the free energy density and on the appearance of ordering, are also discussed.

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CONTENTS

I. INTRODUCTION AND OVERVIEW

Understanding what differentiates the collective behavior of a large quantum system from that of its classical counterpart is a challenging problem of theoretical physics. An important example here is a phase transition, due to which the system becomes ordered in one or another way. Intuitively, it is clear that intrinsic randomness of quantum systems should enhance thermal fluctuations in their work against ordering. For the most of realistic models, the theoretical explanation of such quantum effects is typically based on additional simplifications and uncontrolled approximations. However, as we show in this article, for a certain class of important realistic quantum models a rigorous mathematical theory based on the so called 'first principles' can be developed in detail, qualitatively agreeing with relevant experimental data. These models are *quantum anharmonic crystals*, used, e.g., in the theory of structural phase transitions in solids triggered by the ordering of light particles. At low temperatures, the mentioned quantum effects prevent such light particles from ordering and thus stabilize the crystal. We call this effect *quantum stabilization*, see (Albeverio *et al.*, 2003a). Its mathematical description is based on the use of infinite dimensional (path) integrals and the corresponding path measures, which serve here as mathematical models of thermodynamic phases. This allows us to apply powerful tools of modern mathematical analysis, which, however, makes the theory quite involved. The purpose of the present article is to explain the main aspects of this theory in the way accessible also to non-mathematicians. We do this by interpreting the corresponding ideas and results published in our recent monograph (Albeverio *et al.*, 2009). As we aim at reviewing the results, but not the literature, the quotations are restricted to a necessary minimum. The reader interested in the bibliography on this topic is cordially invited to find it in the Bibliographic Notes to each chapter of (Albeverio *et al.*, 2009).

An anharmonic oscillator is a mathematical model of a point particle moving in a potential field with multiple minima and sufficient growth at infinity, which makes the particle motion confined to the vicinity of the point of its (possibly unstable) equilibrium. In the simplest case, the displacement q of the particle from this point is one-dimensional and the corresponding potential energy $V(q)$ is a symmetric continuous function with two minima at $\pm q_*$, separated by a barrier. In this case, one speaks of *double-well* potentials, an example of which is given in Fig. 1.
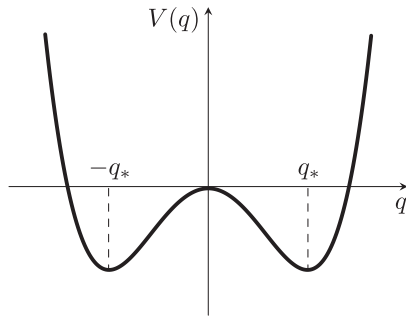
FIG. 1 The case of $V(q) = -\alpha q^2 + bq^4$, α and b strictly positive.

Let now an infinite system of such point particles be arranged into a crystal. That is, each particle is localized in the vicinity of its own crystal site. Suppose also that the particles interact with each other. The corresponding model, called an *anharmonic crystal*, is often used in solid state physics to describe, e.g., ionic crystals containing localized light particles oscillating in the field created by heavy ionic complexes. The ordering of such light particles may trigger a structural change of the whole crystal, see (Bruce and Cowley, 1981). A particular example of this sort can be a KDP-type ferroelectric with hydrogen bounds, in which such light particles are protons or deuterons performing one-dimensional oscillations along the bounds, see (Blinc and Žekš, 1974; Stamenković, 1998; Tokunaga and Matsubara, 1966). Another relevant physical object is a system of apex oxygen ions in YBaCuO-type high-temperature superconductors (Frick *et al.*, 1990; Müller, 1990; Stasyuk, 1999; Stasyuk and Trachenko, 1997). Anharmonic oscillators are also used in models describing the interaction of vibrating particles with a radiation field (Hainzl, 2003; Hirokawa *et al.*, 2005), strong electron-electron correlations caused by the interaction of electrons with vibrating ions (Freericks *et al.*, 1996), or charge transfer along hydrogen bounds (Stasyuk *et al.*, 2002).

If the particle motion obeys the laws of classical mechanics, the low energy states of the particle are degenerate. By this we mean the existence of different states with the same energy, as the particle is confined to one of the wells if its energy is less than the height of the potential barrier separating the wells. Then the low temperature equilibrium thermodynamic states (phases) of the corresponding anharmonic crystal can also be multiple. If this is the case, as the temperature changes the crystal undergoes a phase transition – a collective phenomenon caused by the interaction and by the degeneracy mentioned above. If the particle mass is sufficiently small, it moves according to the laws of quantum mechanics, and hence can tunnel through the potential barrier. This tunneling motion eliminates the degeneracy, which might affect the ability of the phase transition to occur or even suppress it completely. On the theoretical level, such 'quantum effects' were first discussed in (Schneider *et al.*, 1976). Later on, a number of publications on this item appeared, see (Minlos *et al.*, 2002; Stamenković *et al.*, 1987; Verbeure and Zagrebnov, 1993, 1995) and the literature quoted therein. The key conclusion of those works is that the quantum effects become strong whenever the particle mass $m_{\rm ph}$ gets small. This agrees with the experimental data on the isotopic effect in hydrogen bound ferroelectrics (Blinc and Žekš, 1974) and in YBaCuO-type high-temperature superconductors (Müller, 1990). At the same time, experiments show that high hydrostatic pressure applied to a ferroelectric crystal diminishes the phase transition temperature, see, e.g., (Tibballs *et al.*, 1982) and the table on page 11 in (Blinc and Žekš, 1974). Hence, the reduction of the distance between the wells amplifies quantum effects. From this one concludes that also the shape of the localizing potential V plays an important role here.

In the mathematical theory of classical anharmonic crystals, a thermodynamic phase appears as a Gibbs measure defined by a specific condition, involving the potential energy of a single particle and the interaction between the particles. Usually, this condition is formulated as the *Dobrushin-Lanford-Ruelle (DLR) equation* which the Gibbs measures in question have to solve. For quantum infinite particle systems, thermodynamic states are usually described as linear functionals on non-commutative algebras of observables, see (Bratteli and Robinson, 1981). However, for quantum crystals the direct construction of such states appears to be impossible as the relevant observables are unbounded operators. In view of this, the results mentioned above were based on rather indirect indications, e.g., the lack of a symmetry breaking (Verbeure and Zagrebnov, 1993) or of an order parameter (Minlos *et al.*, 2002). It soon had become clear that a mathematical theory, which describes phase transitions and quantum effects in a unified way, and which as well takes into account the role of the localizing potential, ought to be based on a precise definition of thermodynamic phases. Such a theory was elaborated in a series of works, see (Albeverio *et al.*, 1998, 2001, 2002, 2003a,b, 2004; Kargol *et al.*, 2008; Kondratiev and Kozitsky, 2003; Kozitsky, 2002; Kozitsky and Pasurek, 2007; Pasurek, 2008) and the citations therein. The key aspect of this theory is the use of path integral techniques

in which thermodynamic phases are constructed as probability measures on path spaces (path measures) that solve the corresponding DLR equations. Thereafter, necessary and sufficient conditions are derived for a phase transition to occur expressed in terms of the particle mass m_{ph}, the interaction strength $\hat{J}_0$, and a parameter characterizing the potential energy V. In the simplest case where

$$V(q) = -\alpha q^2 + bq^4, \quad \text{and} \quad q_* = \sqrt{\alpha/2b}, \tag{1}$$

cf. Fig.1, both conditions can be expressed through one and the same parameter $Q = (4m_{\mathrm{ph}}/9\hbar^2)q_*^4\hat{J}_0$, and have the following surprisingly simple form: (a) $Q > d\theta(d)$ (sufficient); (b) $Q \geq \varkappa$ (necessary). Here $\theta(d)$ is a certain function of the lattice dimension d, such that $d\theta(d) > 1$ and $d\theta(d) \to 1$ as $d \to +\infty$, see (73) and (74) below. The parameter $\varkappa \leq 1$ is determined by the spectral properties of the single-particle Hamiltonian (6) with $h = 0$, see (94) below.

A self-contained presentation of path integral methods in the statistical mechanics of systems of interacting quantum anharmonic oscillators is given in the monograph (Albeverio *et al.*, 2009), addressed to both communities – mathematicians and physicists. The reader can find here a collection of facts, concepts, and tools relevant for the application of functional-analytic and measure-theoretic methods to problems of quantum statistical mechanics. This includes, in particular, a complete description of the theory mentioned above, as well as of its far-going extensions and implications. In this article based on that monograph, we present and explain some of its details.

II. THE MODEL AND ITS THERMODYNAMICS

A. The model

To be more concrete, we assume that the considered model describes an ionic crystal and thus adopt the ferroelectric terminology. This means that we study a system of light particles oscillating in the field created by ionic complexes, which we suppose to be fixed (adiabatic approximation). A substance modeled in this way might be a KDP type ferroelectric (Blinc and Žekš, 1974; Tokunaga and Matsubara, 1966), in which such particles are protons – ions of hydrogen, constituting hydrogen bounds. Each particle carries an electric charge; hence, its displacement from equilibrium produces a dipole moment, proportional to the displacement. Therefore, the main contribution to the interaction between two particles is proportional to the product of their displacements. According to these arguments, our model is described by the Hamiltonian

$$H = -\frac{1}{2}\sum_{x,y} J_{xy}(q_x, q_y) + \sum_x H_x. \tag{2}$$

Here the sums run through a crystalline lattice, which we assume to be a d-dimensional 'hypercubic' lattice $\mathbb{Z}^d$ consisting of vectors $x = (x_1, \ldots, x_d)$, $x_i \in \mathbb{Z}$, and $\mathbb{Z}$ being the set of all (positive and non-positive) integers. The displacement q_x of the particle localized near such $x = (x_1, \ldots, x_d)$ is supposed to be a ν-dimensional vector, i.e., $q_x = (q_x^{(1)}, \ldots, q_x^{(\nu)})$ and

$$(q_x, q_y) = \sum_{j=1}^{\nu} q_x^{(j)} q_y^{(j)} \tag{3}$$

stands for the corresponding scalar product. Regarding the interaction intensities J_{xy}, we suppose that there exists a real-valued function φ such that

$$J_{xy} = \varphi(|x_1 - y_1|, \ldots, |x_d - y_d|). \tag{4}$$

We say that the interaction has *finite range* if φ vanishes whenever either of its arguments exceeds a certain value. In particular, φ can be nonzero only if one of its arguments is equal to one and all other arguments are equal to zero. This is the case of a *nearest neighbor interaction*. To avoid unnecessary mathematical complications, in this article we suppose that J_{xy} has finite range. Note, however, that in (Albeverio *et al.*, 2009) we consider the general case with the only assumption that

$$\hat{J}_0 := \sum_{y \in \mathbb{Z}^d} |J_{xy}| < \infty, \tag{5}$$

see also (Kozitsky and Pasurek, 2007). In addition, we suppose that $J_{xy} \geq 0$, which means that we consider ferroelectric interactions only. The single-particle Hamiltonian in (2) has the following form

$$H_x = \frac{1}{2m}|p_x|^2 + V(q_x) - (h, q_x) \tag{6}$$

$$= H_x^{\mathrm{har}} + U(q_x) - (h, q_x),$$

where $h \in \mathbb{R}^\nu$ is an external (electric) field,

$$H_x^{\mathrm{har}} = \frac{1}{2m}|p_x|^2 + \frac{a}{2}|q_x|^2, \tag{7}$$

is the Hamiltonian of a harmonic oscillator of rigidity $a > 0$, and

$$U(q_x) = V(q_x) - \frac{a}{2}|q_x|^2, \tag{8}$$

is the anharmonic part of the potential energy V. For the sake of convenience, we exclude from the latter the external field term. One observes that H_x as given in (6) is independent of the choice of x; thus, the model (2) is invariant under the translations of the lattice $\mathbb{Z}^d$. The mass parameter m in (6) and (7) includes Planck's constant, i.e.,

$$m = m_{\mathrm{ph}}/\hbar^2. \tag{9}$$

The Hamiltonian (6) is defined as a linear operator acting in the 'physical' complex Hilbert space $\mathcal{H}_x = L^2(\mathbb{R}^\nu)$ of square-integrable 'wave' functions, which have the standard physical interpretation. In particular, for $\psi \in \mathcal{H}_x$ such that

$$\|\psi\|_{\mathcal{H}_x}^2 := \int_{\mathbb{R}^\nu} |\psi(u)|^2 du = 1,$$

and for a bounded linear operator $A : \mathcal{H}_x \to \mathcal{H}_x$, the (complex) number

$$\omega_\psi(A) := (\psi, A\psi)_{\mathcal{H}_x} = \int_{\mathbb{R}^\nu} \bar{\psi}(u)(A\psi)(u) du \tag{10}$$

is said to be the value of A in vector state ω_ψ. Here

$$(\phi, \psi)_{\mathcal{H}_x} = \int_{\mathbb{R}^\nu} \bar{\phi}(u)\psi(u) du, \qquad \phi, \psi \in \mathcal{H}_x,$$

is the scalar product in $\mathcal{H}_x$, and $\bar{\phi}$ stands for the complex conjugate. In general, a *state*, ω, is a map defined on the algebra $\mathfrak{C}_x$ of bounded linear operators $A : \mathcal{H}_x \to \mathcal{H}_x$ with values in the set of complex numbers $\mathbb{C}$ such that, for all $\varsigma_1, \varsigma_2 \in \mathbb{C}$ and all operators $A_1, A_2 \in \mathfrak{C}_x$,

$$\omega(\varsigma_1 A_1 + \varsigma_2 A_2) = \varsigma_1 \omega(A_1) + \varsigma_2 \omega(A_2), \tag{11}$$

$$\omega(I) = 1, \quad \omega(A) \geq 0 \quad \text{for} \quad A \geq 0.$$

Here I is the identity operator and $A \geq 0$ means that $(\psi, A\psi)_{\mathcal{H}_x} \geq 0$ for all $\psi \in \mathcal{H}_x$. Let ω_1 and ω_2 be two states. For $\varsigma \in [0, 1]$, we set

$$\omega = \varsigma\omega_1 + (1 - \varsigma)\omega_2. \tag{12}$$

Then ω is also a states, which is a convex combination (*mixture*) of ω_1 and ω_2. The combination in (12) is called nontrivial, if $\omega \neq \omega_1$ and $\omega \neq \omega_2$. By definition, a pure state is a state which cannot be decomposed into a nontrivial convex combination of other states. Vector states (10) are pure, see Theorem 1.1.15, page 26 in (Albeverio *et al.*, 2009).

In the sequel, we mostly consider the following versions of the model (2), (6):

(i) the dimension ν is arbitrary and V has the form
cf. (1),

$$V(q) = -\alpha|q|^2 + b|q|^4, \qquad \alpha, b > 0; \tag{13}$$

(ii) $\nu = 1$ and V is an even continuous function
    such that, for $|q| < |\tilde{q}|$,

$$W(q) - V(q) \leq W(\tilde{q}) - V(\tilde{q}), \tag{14}$$

where

$$W(q) = -b_1 q^2 + \sum_{l=2}^{r} b_l q^{2l}, \tag{15}$$

$$b_1, b_r > 0, \quad b_l \geq 0, \text{ for } l = 2, \ldots, r-1,$$

and $r \geq 2$ is a finite integer;

(iii) $\nu = 1$ and V is continuous, asymmetric, i.e.,
    $V(q) \neq V(-q)$, and such that the following
    estimate holds

$$V(q) \geq -C + D|q|^{2+\epsilon}, \quad q \in \mathbb{R}, \tag{16}$$

where C, D, and ϵ are positive constants.

Assuming that V in (14) is differentiable, we can rewrite this condition in the form

$$-b_1 + \sum_{l=2}^{r} l b_l \vartheta^{l-1} \geq v'(\vartheta), \qquad \text{for all } \vartheta > 0,$$

where v is such that $V(q) = v(q^2)$. Along with the function W we also use

$$\Phi(\vartheta) = \sum_{l=2}^{r} \frac{(2l)!}{2^{l-1}(l-1)!} b_l \vartheta^l, \quad \vartheta \geq 0, \tag{17}$$

where r and all b_l are the same as in (15). One observes that in cases (i) and (ii) with $h = 0$, the model is $O(\nu)$-symmetric, that is, it is symmetric with respect to all orthogonal transformations of $\mathbb{R}^\nu$, which constitute the group[1] $O(\nu)$. Then the phase transition in the corresponding model can be associated with the breakdown of this symmetry. Case (iii) is essentially different from this point of view.

We conclude this subsection by recalling that the Hamiltonian in (2) corresponds to a quantum model. In particular, this means that p_x and q_x are (unbounded) operators, which in view of (9) obey the following commutation relations

$$p_x^{(j)} q_y^{(j')} - q_y^{(j')} p_x^{(j)} = -\mathrm{i}\delta_{xy}\delta_{jj'}, \qquad \mathrm{i} = \sqrt{-1}. \tag{18}$$

B. A single anharmonic oscillator

As we shall see below, important thermodynamic properties of the model (2) are closely related to the quantum-mechanical properties of the anharmonic oscillator described by the Hamiltonian (6), in which we set $h = 0$. To avoid nonessential technical problems, we suppose that V in (6) is an $O(\nu)$-symmetric polynomial and thus is of the following form

$$V(q) = \sum_{l=1}^{r} c_l |q|^{2l}, \qquad c_r > 0, \tag{19}$$

with $r \geq 1$, cf. (13). This, of course, includes also the case of the harmonic oscillator (7). For such V, there exists a subset $\mathcal{D}$ of the physical Hilbert space $\mathcal{H}_x$ such that H_x with domain $\mathcal{D}$ is a self-adjoint operator, see Theorem 1.1.47,

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[1] Note that the only nontrivial transformation in $O(1)$ is $q \mapsto -q$.

page 46 in (Albeverio *et al.*, 2009). Its spectrum consists entirely of real eigenvalues E_n, $n \in \mathbb{N}_0$, such that, for some $E_* > 0$ and $n_* \in \mathbb{N}$, they obey the estimate

$$E_n \geq E_* n^{2r/(r+1)}, \qquad \text{for all} \;\; n \geq n_*,$$

see Theorem 1.1.58, page 53 in (Albeverio *et al.*, 2009). In particular, the eigenvalues E_n^{har}, $n \in \mathbb{N}_0$, of H_x^{har}, are

$$E_n^{\text{har}} = (n + \nu/2)\Delta^{\text{har}}, \qquad \Delta^{\text{har}} := \sqrt{a/m}, \tag{20}$$

see e.g. Proposition 1.1.37, page 41 in (Albeverio *et al.*, 2009). If $\nu = 1$, the eigenvalues E_n are simple, which means that, for every $n \in \mathbb{N}_0$, the equation

$$H_x \psi_n = E_n \psi_n$$

has exactly one solution $\psi_n \in \mathcal{H}_x$. The dynamical properties of the oscillator crucially depend on the following *gap* parameter

$$\Delta = \inf_{n \in \mathbb{N}_0} (E_{n+1} - E_n). \tag{21}$$

Note that

$$\Delta \to 0, \qquad \text{as} \;\; m \to +\infty. \tag{22}$$

The latter, in fact, is the classical limit $\hbar \to 0$, see (9). It can be shown that, for a fixed value of the mass parameter m,

$$\lim_{n \to +\infty} (E_{n+1} - E_n) = +\infty. \tag{23}$$

Thus, the infimum in (21) is strictly positive for finite values of m. As usual, for appropriate functions f and g, by writing $f \sim g$ we mean that $\lim(f/g) = 1$ assuming that the meaning of the limit is clear from the context. In the harmonic case, the gap parameter is given in (20). According to Theorem 1.1.60, page 59 in (Albeverio *et al.*, 2009), Δ is a continuous function of the mass parameter $m > 0$ such that, cf. (22),

$$\Delta \sim \Delta_0 m^{-r/(r+1)}, \qquad \text{as} \;\; m \to 0, \tag{24}$$

where r is the same as in (19) and (15). The proof of these properties goes as follows. First, by the analytic perturbation theory for self-adjoint operators one shows that the eigenvalues E_n, and hence the increments $E_{n+1} - E_n$, continuously depend on m. This, however, does not yet mean the continuity of Δ, as the infimum of an infinite number of continuous functions need not be continuous. But, by (23) we see that, for some $n_0 \in \mathbb{N}$,

$$E_{n+1} - E_n > E_{k+1} - E_k$$

for any $n > n_0$ and any $k < n_0$. This means that the infimum in (21) can be found by means of a finite number of increments, i.e.,

$$\Delta = \min_{n=0,1,\ldots,n_0} (E_{n+1} - E_n),$$

which yields the continuity in question. Finally, the asymptotics (24) is obtained by means of a rescaling and then by the asymptotic perturbation theory for self-adjoint operators. From this we conclude that the following parameter

$$R_m := m\Delta^2 \tag{25}$$

is a continuous function of m and

$$R_m \sim \Delta_0^2 m^{-(r-1)/(r+1)}, \qquad \text{as} \;\; m \to 0. \tag{26}$$

Noteworthy, R_m, $\hat{J}_0$ as given in (5), and the rigidity a as in (7), are measured in the same physical units, cf. (9). We also note that $R_m \to 0$ in the classical limit $m \to +\infty$, see (93) below. In the harmonic case, $R_m^{\text{har}} = a$, see (20). By analogy, we call R_m the *quantum rigidity* of the oscillator described by H_x. By the mentioned continuity and by (26), for $r \geq 2$, R_m takes any value from an interval $[R^{(0)}, +\infty)$ for some $R^{(0)} > 0$. As we shall see below, for big enough values of R_m, phase transitions in the model (2) are suppressed at all temperatures.

C. Thermodynamic phases

The Hamiltonian given in (2) has no direct mathematical meaning and serves as a formula for 'local' Hamiltonians

$$H_\Lambda = -\frac{1}{2} \sum_{x,y \in \Lambda} J_{xy}(q_x, q_y) + \sum_{x \in \Lambda} H_x, \tag{27}$$

indexed by finite subsets $\Lambda \subset \mathbb{Z}^d$. Let $|\Lambda|$ stand for the number of lattice sites contained in Λ. Then the corresponding physical Hilbert space is $\mathcal{H}_\Lambda = L^2((\mathbb{R}^\nu)^{|\Lambda|})$. Among all linear operators acting in $\mathcal{H}_\Lambda$, we distinguish bounded operators $A : \mathcal{H}_\Lambda \to \mathcal{H}_\Lambda$. The set of all such operators $\mathfrak{C}_\Lambda$ is a C^*-algebra, see Sections 1.1 and 1.2 in (Albeverio *et al.*, 2009) for more information on this topic. The local Hamiltonian defined in (27) is an unbounded operator. However, by the assumptions made above H_Λ is a self-adjoint operator on some domain $\mathcal{D}_\Lambda \subset \mathcal{H}_\Lambda$. Moreover, one can show that, for any $\beta > 0$, the operator $\exp(-\beta H_\Lambda)$ has finite trace, and hence the local partition function

$$Z_\Lambda := \operatorname{trace} \exp(-\beta H_\Lambda), \tag{28}$$

is well-defined. Along with the Hamiltonian (27) we will use 'periodic' Hamiltonians defined as follows. Let Λ_L, $L \in \mathbb{N}$, be the subset of the lattice $\mathbb{Z}^d$ consisting of all $x = (x_1, \ldots, x_d)$ such that $-L < x_i \leq L$, for all $i = 1, \ldots, d$. For x_i and y_i, obeying the latter condition, we set

$$|x_i - y_i|_L = \min\{|x_i - y_i|; 2L - |x_i - y_i|\}.$$

Clearly, Λ_L is a cube, which one can turn into a torus by identifying its opposite walls. We denote it also by Λ_L and equip with the distance

$$|x - y|_L = \sqrt{|x_1 - y_1|_L^2 + \cdots + |x_d - y_d|_L^2}. \tag{29}$$

After that, Λ_L becomes invariant with respect to the corresponding translations. Now we introduce

$$J_{xy}^L = \varphi(|x_1 - y_1|_L, \ldots, |x_d - y_d|_L), \quad x, y \in \Lambda_L,$$

where φ is as in (4). Then the periodic Hamiltonian in Λ_L is

$$H_L = -\frac{1}{2} \sum_{x,y \in \Lambda_L} J_{xy}^L(q_x, q_y) + \sum_{x \in \Lambda_L} H_x. \tag{30}$$

Like the Hamiltonian in (27), it is a self-adjoint operator in the corresponding space $\mathcal{H}_{\Lambda_L}$, for which

$$Z_L := \operatorname{trace} \exp(-\beta H_L) < \infty. \tag{31}$$

The local Gibbs state ϱ_Λ at temperature $T = 1/\beta k_B$, k_B being Boltzmann's constant, is defined to be

$$\varrho_\Lambda(A) = \operatorname{trace}\{A \exp(-\beta H_\Lambda)\}/Z_\Lambda, \quad A \in \mathfrak{C}_\Lambda. \tag{32}$$

It is a positive linear functional on the algebra $\mathfrak{C}_\Lambda$, cf. (11). Moreover, it is the following mixture, cf. (12),

$$\varrho_\Lambda = \frac{1}{Z_\Lambda} \sum_{n=0}^{\infty} \exp\left(-\beta E_\Lambda^{(n)}\right) \omega_{\psi_n}$$

of the vector states ω_{ψ_n} corresponding to the eigenvectors of H_Λ defined by

$$H_\Lambda \psi_n = E_\Lambda^{(n)} \psi_n.$$

In the same way, we define the periodic local state

$$\varrho_L(A) = \operatorname{trace}\{A \exp(-\beta H_L)\}/Z_L, \quad A \in \mathfrak{C}_\Lambda. \tag{33}$$

If not explicitly stated otherwise, all properties of the states ϱ_Λ that we mention in the sequel are attributed also to the periodic states ϱ_L.

By Høegh-Krohn's theorem, see page 72 in (Albeverio *et al.*, 2009), ϱ_Λ can be recovered from its values on the products of the form

$$\mathfrak{a}_{t_1}^\Lambda(F_1)\cdots\mathfrak{a}_{t_n}^\Lambda(F_n),\quad n\in\mathbb{N},$$

$$F_1,\ldots,F_n\in\mathfrak{F}_\Lambda,\qquad t_1,\ldots,t_n\in\mathbb{R},$$

where $\mathfrak{F}_\Lambda$ is a 'rich enough' family of multiplication operators by bounded measurable functions $F:\mathbb{R}^{|\Lambda|}\to\mathbb{C}$. Here

$$\mathfrak{a}_t^\Lambda(A)=\exp(itH_\Lambda)A\exp(-itH_\Lambda),\qquad A\in\mathfrak{C}_\Lambda,$$

is the time automorphism $\mathfrak{a}_t^\Lambda:\mathfrak{C}_\Lambda\to\mathfrak{C}_\Lambda$ which in the Heisenberg approach describes the dynamics of the oscillators located in Λ. Thus, the Green functions

$$G_{F_1,\ldots,F_n}(t_1,\ldots,t_n):=\varrho_\Lambda\left[\mathfrak{a}_{t_1}^\Lambda(F_1)\cdots\mathfrak{a}_{t_n}^\Lambda(F_n)\right],\tag{34}$$

with all possible choices of $n\in\mathbb{N}$ and then of $F_1,\ldots,F_n\in\mathfrak{F}_\Lambda$ determine the state ϱ_Λ. Each Green function admits an analytic continuation, also denoted by $G_{F_1,\ldots,F_n}$, to the domain D_n consisting of those $(\zeta_1,\ldots,\zeta_n)\in\mathbb{C}^n$, for which

$$0<\mathrm{Im}(\zeta_1)<\cdots<\mathrm{Im}(\zeta_n)<\beta.$$

Furthermore, see Theorem 1.2.32, page 78 in (Albeverio *et al.*, 2009), $G_{F_1,\ldots,F_n}$ is continuous on the closure $\overline{D}_n$ and can uniquely be recovered from its restriction to the set

$$D_n^{(0)}:=\{(\zeta_1,\ldots,\zeta_n)\in\overline{\mathcal{D}}_n:\mathrm{Re}(\zeta_1)=\cdots=\mathrm{Re}(\zeta_n)=0\}.$$

Thus, the Matsubara functions

$$\Gamma_{F_1,\ldots,F_n}(\tau_1,\ldots,\tau_n):=G_{F_1,\ldots,F_n}(i\tau_1,\ldots,i\tau_n),\tag{35}$$

with

$$0\le\tau_1\le\tau_2\cdots\le\tau_n\le\beta,\tag{36}$$

and with all possible choices of $n\in\mathbb{N}$ and then of $F_1,\ldots,F_n\in\mathfrak{F}_\Lambda$, uniquely determine the state (32). By (34), we can rewrite (35) in the form

$$\Gamma_{F_1,\ldots,F_n}(\tau_1,\ldots,\tau_n)=\mathrm{trace}\left[F_1e^{-(\tau_2-\tau_1)H_\Lambda}F_2e^{-(\tau_3-\tau_2)H_\Lambda}\cdots F_ne^{-(\tau_{n+1}-\tau_n)H_\Lambda}\right]/Z_\Lambda,\tag{37}$$

where $\tau_{n+1}=\beta+\tau_1$ and the arguments obey (36). The main ingredient of our technique is the following representation, see Theorem 1.4.5 in (Albeverio *et al.*, 2009),

$$\Gamma_{F_1,\ldots,F_n}(\tau_1,\ldots,\tau_n)\tag{38}$$

$$=\int_{\Omega_\Lambda}F_1(\omega_\Lambda(\tau_1))\cdots F_n(\omega_\Lambda(\tau_n))\nu_\Lambda(d\omega_\Lambda),$$

where ν_Λ is the 'local Euclidean Gibbs measure' in Λ, which is a probability measure on the measurable space $(\Omega_\Lambda,\mathcal{B}(\Omega_\Lambda))$. Here

$$\Omega_\Lambda:=\{\omega_\Lambda=(\omega_x)_{x\in\Lambda}:\omega_x\in C_\beta\},$$

$$C_\beta:=\{\phi\in C([0,\beta]\to\mathbb{R}^\nu):\phi(0)=\phi(\beta)\},$$

and $C([0,\beta]\to\mathbb{R}^\nu)$ stands for the set of all continuous functions (paths) $\phi:[0,\beta]\to\mathbb{R}^\nu$, also called 'continuous temperature loops' in view of the periodicity property $\phi(0)=\phi(\beta)$. Thus, C_β is the Banach space of paths. The space Ω_Λ is equipped with the corresponding product topology and with the Borel σ-field $\mathcal{B}(\Omega_\Lambda)$. The measure ν_Λ has the following Feynman-Kac representation

$$\nu_\Lambda(d\omega_\Lambda)=\exp\left[-I_\Lambda(\omega_\Lambda)\right]\chi_\Lambda(d\omega_\Lambda)/N_\Lambda(h),\tag{39}$$

in which

$$I_\Lambda(\omega_\Lambda) = -\frac{1}{2} \sum_{x,y\in\Lambda} J_{xy} \int_0^\beta (\omega_x(\tau), \omega_y(\tau)) d\tau \tag{40}$$

$$- \sum_{x\in\Lambda} \int_0^\beta (h, \omega_x(\tau)) d\tau + \sum_{x\in\Lambda} \int_0^\beta U(\omega_x(\tau)) d\tau$$

is the energy functional. We recall that U in (40) is the anharmonic part of V, see (8), and that, for each τ and x, $\omega_x(\tau)$ is a ν-dimensional vector and thus $(\cdot, \cdot)$ in (40) stands for the corresponding scalar product, cf. (3). The normalizing term $N_\Lambda(h)$ is defined by the condition

$$N_\Lambda(h) = \int_{\Omega_\Lambda} \exp\left[-I_\Lambda(\omega_\Lambda)\right] \chi_\Lambda(d\omega_\Lambda), \tag{41}$$

and the measure χ_Λ has the form

$$\chi_\Lambda(d\omega_\Lambda) = \prod_{x\in\Lambda} \chi(d\omega_x). \tag{42}$$

Here χ is the Høegh-Krohn measure – a Gaussian probability measure on the Banach space C_β, constructed by means of the harmonic part of the Hamiltonian (6). It is defined by its Fourier transform

$$\int_{C_\beta} \exp\left(i \sum_{j=1}^\nu \int_0^\beta \lambda^{(j)}(\tau) \omega_x^{(j)}(\tau) d\tau\right) \chi(d\omega_x) = \exp\left(-\frac{1}{2} \sum_{j=1}^\nu \int_0^\beta \int_0^\beta S(\tau, \tau') \lambda^{(j)}(\tau) \lambda^{(j)}(\tau') d\tau d\tau'\right),$$

where λ is in C_β and $S(\tau, \tau')$ is the *propagator* corresponding to a single scalar ($\nu = 1$) harmonic oscillator, which, in fact, is the corresponding Matsubara function (35) for $n = 2$ and $F_1 = F_2 = q_x$. That is, cf. (37), (7), and (20),

$$S(\tau, \tau') = \frac{1}{Z^{\text{har}}} \text{trace}\left[q_x \exp\left(-|\tau' - \tau| H_x^{\text{har}}\right) q_x \exp\left(-(\beta - |\tau' - \tau|) H_x^{\text{har}}\right)\right] \tag{43}$$

$$= \left[\exp\left(-|\tau' - \tau|\Delta^{\text{har}}\right) + \exp\left(-(\beta - |\tau' - \tau|)\Delta^{\text{har}}\right)\right] \Big/ 2\sqrt{ma}\left[1 - \exp\left(-\beta\Delta^{\text{har}}\right)\right],$$

see pages 99 and 125 in (Albeverio *et al.*, 2009). In a similar way, one defines also periodic local Gibbs measures, cf. (30),

$$\nu_L(d\omega_{\Lambda_L}) = \exp\left[-I_L(\omega_{\Lambda_L})\right] \chi_{\Lambda_L}(d\omega_{\Lambda_L})/N_L(h), \tag{44}$$

with

$$N_L(h) = \int_{\Omega_{\Lambda_L}} \exp\left[-I_L(\omega_{\Lambda_L})\right] \chi_{\Lambda_L}(d\omega_{\Lambda_L}), \tag{45}$$

and

$$I_L(\omega_{\Lambda_L}) = -\frac{1}{2} \sum_{x,y\in\Lambda_L} J_{xy}^L \int_0^\beta (\omega_x(\tau), \omega_y(\tau)) d\tau$$

$$- \sum_{x\in\Lambda_L} \int_0^\beta (h, \omega_x(\tau)) d\tau + \sum_{x\in\Lambda_L} \int_0^\beta U(\omega_x(\tau)) d\tau.$$

Thus, the representation (38) leads to the description of the states (32), (33) in terms of Gibbs measures, similarly as in the case of classical anharmonic crystals. Here, however, each ν-dimensional vector q_x is replaced by a continuous ν-dimensional path ω_x, which is an element of an infinite dimensional vector space. Going further in this direction, one can define 'global' Gibbs states of the model (2) as the probability measures on the space of 'tempered configurations' satisfying the DLR equation, see Chapter 3 in (Albeverio *et al.*, 2009). It can be shown that the set of all such

measures, which we denote by $\mathcal{G}$, is a nonempty compact simplex with a nonempty extreme boundary $\mathrm{ex}(\mathcal{G})$, the elements of which correspond to the *thermodynamic phases* of our model, see also Chapter 7 in (Georgii, 1988). Thus, by a thermodynamic phase we understand an extreme element of $\mathcal{G}$. The latter means that such a measure cannot be decomposed into a nontrivial convex combination of other elements of $\mathcal{G}$. By virtue of the DLR equation, the set $\mathcal{G}$ can contain either one or infinitely many elements. Correspondingly, the multiplicity (resp. the uniqueness) of thermodynamic phases existing at a given value of the temperature means that $|\mathrm{ex}(\mathcal{G})| > 1$ (resp. $|\mathcal{G}| = 1$). In general, there exist several ways of establishing whether the set of Gibbs measures is infinite or containing a single element. One of them consists in showing that there exists an element of $\mathcal{G}$, which is 'less symmetric' than the corresponding Hamiltonian, i.e., that a symmetry breaking occurs. Another way is to show that $\mathcal{G}$ contains an element, which is not in $\mathrm{ex}(\mathcal{G})$. Since the latter is a subset of $\mathcal{G}$, then $\mathcal{G}$ is not a singleton, and hence $|\mathcal{G}| = +\infty$. The latter way will be discussed below in more detail.

D. The free energy

A more 'traditional' way of establishing phase transitions is based on the use of thermodynamic functions. In our case, this will be the free energy. Recall that we assume J_{xy} to be of finite range. Along with the energy functional (40) we consider also

$$I_\Lambda(\omega_\Lambda|\xi) = I_\Lambda(\omega_\Lambda) \tag{46}$$

$$- \sum_{x\in\Lambda,\ y\in\Lambda^c} J_{xy} \int_0^\beta (\omega_x(\tau), \xi_y(\tau))d\tau,$$

where $I_\Lambda(\omega_\Lambda)$ is as in (40) and all ξ_y with $y \in \Lambda^c := \mathbb{Z}^d \setminus \Lambda$, belong to C_β. The last term in (46) describes the interaction of the particles in Λ with some 'environment' defined by the configuration ξ fixed outside Λ. We recall that $I_\Lambda(\omega_\Lambda)$ depends on the external field parameter $h \in \mathbb{R}^d$. For χ_Λ as in (42), we set

$$N_\Lambda(h,\xi) = \int_{\Omega_\Lambda} \exp\left[-I_\Lambda(\omega_\Lambda|\xi)\right] \chi_\Lambda(d\omega_\Lambda),$$

which is well-defined as J_{xy} has finite range, and hence the sum in (46) is finite. Obviously, if $\xi_y \equiv 0$ for all $y \in \Lambda^c$, then the above $N_\Lambda(h,\xi)$ coincides with $N_\Lambda(h)$ given in (41). We also note that the partition function (28) and $N_\Lambda(h)$ are related to each other by

$$Z_\Lambda = N_\Lambda(h) Z_\Lambda^{\mathrm{har}}, \tag{47}$$

where Z_Λ^{har} is the partition function of the system of non-interacting harmonic oscillators located in Λ. Explicit calculations yield, see page 139 in (Albeverio *et al.*, 2009),

$$Z_\Lambda^{\mathrm{har}} = \left[\mathrm{trace}\exp\left(-\beta H_x^{\mathrm{har}}\right)\right]^{|\Lambda|}$$

$$= \left[\frac{e^{-\beta\Delta^{\mathrm{har}}/2}}{1 - e^{-\beta\Delta^{\mathrm{har}}}}\right]^{\nu|\Lambda|},$$

where $\Delta^{\mathrm{har}} = \sqrt{a/m}$ is the same as in (20) and (43). In a similar way, we have

$$Z_L = N_L(h) Z_\Lambda^{\mathrm{har}}, \tag{48}$$

where Z_L and $N_L(h)$ are as in (31) and (45), respectively. Therefore, $N_L(h)$, $N_\Lambda(h)$, and $N_\Lambda(h,\xi)$ are relative partition functions, and the latter one corresponds to the system of particles in Λ interacting with the 'environmental' configuration ξ. Let us now define

$$F_\Lambda(h,\xi) = -\frac{1}{\beta|\Lambda|} \ln N_\Lambda(h,\xi), \tag{49}$$

$$F_\Lambda(h) = -\frac{1}{\beta|\Lambda|} \ln N_\Lambda(h),$$

and

$$F_L(h) = -\frac{1}{\beta|\Lambda_L|}\ln N_L(h). \tag{50}$$

Note that $F_\Lambda(h) = F_\Lambda(h,0)$ and $|\Lambda_L| = (2L)^d$. The functions just introduced are called *local free energy densities*. For a Gibbs measure $\mu \in \mathcal{G}$, we then set

$$F_\Lambda^\mu(h) = \int_\Omega F_\Lambda(h,\xi)\mu(d\xi). \tag{51}$$

This is the free energy density of the system of particles in Λ, interacting with the environment averaged with respect to μ. In the following, we are interested in the thermodynamic limits of the functions (49) – (51). To define such limits, we need one more notion which we introduce now. Let Λ be a finite subset of $\mathbb{Z}^d$. We say that $y \in \mathbb{Z}^d$ is a *neighbor* of Λ if: (a) y is not in Λ, i.e., $y \in \Lambda^c$; (b) there exists $x \in \Lambda$ such that x and y are neighbors, i.e.,

$$|x - y| = \sqrt{|x_1 - y_1|^2 + \cdots + |x_d - y_d|^2} = 1.$$

By $\partial\Lambda$ we denote the set of all neighbors of Λ, $|\partial\Lambda|$ standing for their number. A sequence $\{\Lambda_n\}_{n\in\mathbb{N}}$ of finite subsets of $\mathbb{Z}^d$ is said to be a *van Hove sequence*, cf. page 193 in (Albeverio *et al.*, 2009), if: (a) $\Lambda_n \subset \Lambda_{n+1}$ for every $n \in \mathbb{N}$; (b) for every $y \in \mathbb{Z}^d$, one finds n such that $y \in \Lambda_n$; (c) $\lim_{n\to+\infty} |\partial\Lambda_n|/|\Lambda_n| = 0$. An example of such a sequence can be the sequence of cubes Λ_{L_n} for any strictly increasing sequence of positive integers L_n. For a van Hove sequence $\{\Lambda_n\}_{n\in\mathbb{N}}$, we denote

$$F(h) = \lim_{n\to+\infty} F_{\Lambda_n}(h), \quad F^\mu(h) = \lim_{n\to+\infty} F_{\Lambda_n}^\mu(h), \tag{52}$$

where $F_{\Lambda_n}(h)$ and $F_{\Lambda_n}^\mu(h)$ are as in (49) and (51), respectively. Furthermore, for a strictly increasing sequence $\{L_n\}$ and $F_{L_n}(h)$ as in (50), we set

$$F^{\mathrm{per}}(h) = \lim_{n\to+\infty} F_{L_n}(h). \tag{53}$$

It is known, see Theorem 5.1.3 on page 268 in (Albeverio *et al.*, 2009), that, for any $\mu \in \mathcal{G}$ and for any van Hove sequence $\{\Lambda_n\}_{n\in\mathbb{N}}$, both limits in (52) exist, do not depend on the choice of $\{\Lambda_n\}_{n\in\mathbb{N}}$, and are equal to each other. Furthermore, for any sequence $\{L_n\}_{n\in\mathbb{N}}$ such that $L_n \to +\infty$, the limit in (53) exists, is independent of the choice of $\{L_n\}_{n\in\mathbb{N}}$, and is equal to the limits in (52). That is,

$$F^{\mathrm{per}}(h) = F(h) = F^\mu(h), \qquad \text{for all } \mu \in \mathcal{G}. \tag{54}$$

Therefore, $F(h)$ is a universal thermodynamic function characterizing the model, that along with h depends also on β. Note that in (Albeverio *et al.*, 2009), instead of $F(h)$ we considered the *pressure* $p(h) = -\beta F(h)$.

We recall that the model (2) with $\nu > 1$ is considered only with V as in (i). In this case the free energy density depends only on the norm of the external field, which we can choose therefore in the form $(h, 0, \ldots, 0)$ with $h \in \mathbb{R}$. In the remaining (ii) and (iii) cases, we have $\nu = 1$ and hence $h \in \mathbb{R}$. Thus, from now on we assume that $h \in \mathbb{R}$ in all cases. By (49), (41), and (47), we obtain

$$-\frac{\partial}{\partial h}F_\Lambda(h) = -\frac{1}{\beta|\Lambda|}\frac{\partial}{\partial h}Z_\Lambda \tag{55}$$

$$= \frac{1}{|\Lambda|}\sum_{x\in\Lambda}\varrho_\Lambda[q_x^{(1)}] =: M_\Lambda(h).$$

Here $M_\Lambda(h)$ is the *local polarization* averaged over Λ. Likewise,

$$-\frac{\partial}{\partial h}F_L(h) = -\frac{1}{\beta|\Lambda|}\frac{\partial}{\partial h}Z_L \tag{56}$$

$$= \frac{1}{|\Lambda|}\sum_{x\in\Lambda_L}\varrho_L[q_x^{(1)}] = \varrho_L[q_x^{(1)}] =: M_L(h).$$

Here we have taken into account that the periodic state ϱ_L is invariant with respect to translations of the torus Λ_L. The formulas just obtained relate the local free energy densities with the local polarizations. However, the convergence in (52) and (53) need not yield the convergence of the derivatives, i.e., of the local polarizations. Computing one more derivative in (55) we obtain, see page 220 in (Albeverio *et al.*, 2009),

$$-\frac{\partial^2}{\partial h^2} F_\Lambda(h) = \frac{1}{2\beta|\Lambda|} \int_{\Omega_\Lambda} \int_{\Omega_\Lambda} \left[\sum_{x \in \Lambda} \int_0^\beta (\omega_x(\tau) - \tilde{\omega}_x(\tau)) \, d\tau \right]^2 \nu_\Lambda(d\omega_\Lambda) \nu_\Lambda(d\tilde{\omega}_\Lambda) \geq 0. \tag{57}$$

The latter inequality follows from the fact that we integrate a nonnegative expression, i.e., $[\cdots]^2$. From this inequality we see that F_Λ is a concave function of h. The same is true also for F_L. Thus, the limiting free energy density given in (52) is also a concave function of h. Concave functions always have one-sided derivatives

$$M_\pm(h) = - \lim_{\varepsilon \to 0+} \frac{F(h \pm \varepsilon) - F(h)}{\pm \varepsilon}. \tag{58}$$

If $M_+(h) = M_-(h)$, then $F(h)$ is differentiable at this h, and one can speak of the *global polarization*

$$M(h) := M_+(h) = M_-(h) = -F'(h). \tag{59}$$

Given $h_* \in \mathbb{R}$, we say that $M(h_*)$ does not exist if $M_+(h_*) \neq M_-(h_*)$. By the concavity of F, if the global polarization $M(h)$ exists for a given h, it can be obtained as a limit of the sequences of local polarizations (55), (56), which is independent of the choice of the corresponding van Hove sequences $\{\Lambda_n\}$ or $\{L_n\}$. That is,

$$M(h) = \lim_{n \to +\infty} M_{\Lambda_n}(h) = \lim_{n \to +\infty} M_{L_n}(h). \tag{60}$$

Suppose now that, for a given $h_* \in \mathbb{R}$, $F(h)$ is not differentiable at h_*, but is differentiable on the intervals $(h_* - \varepsilon, h_*)$ and $(h_*, h_* + \varepsilon)$ for some $\varepsilon > 0$. Then $M_+(h_*) \neq M_-(h_*)$, i.e., the polarization $M(h)$ is discontinuous (makes a jump) at h_*, which physicists interpret as a phase transition. However, we failed so far to prove that the discontinuity of $M(h)$ implies the multiplicity of phases, i.e., $|\mathrm{ex}(\mathcal{G})| > 1$, even for the simplest versions of the model[2] (2). The converse statement holds true in the following form, see Theorem 5.3.3, page 276 in (Albeverio *et al.*, 2009).

Theorem 1 *For $\nu = 1$, if the free energy density is differentiable in h at a given h_* and β, then the set of Gibbs measures $\mathcal{G}$ is a singleton, and hence there exists only one thermodynamic phase at these β and h_*.*

In the next subsection, we return to the connection of the properties of $F(h)$ with phase transitions.

We conclude this subsection with the following remark. In some cases, it is possible to find values of h where $F(h)$ is differentiable for all β. In particular, see Theorem 5.2.3 on page 273 in (Albeverio *et al.*, 2009), if $\nu = 1, 2$ and V is as in (13), then $F(h)$ is infinitely differentiable at all $h \neq 0$, and hence $M(h)$ exists at all such h. This result follows from a generalization of the celebrated Lee-Yang theorem, see also Theorem 5.2.4 on page 275 in (Albeverio *et al.*, 2009).

E. Phase transitions and order parameters

We recall that according to our definition a phase transition in the model (2) occurs if it has multiple thermodynamic phases existing at the same values of β and h. Mathematically, this means that the set of Gibbs measures $\mathcal{G}$, and hence its extreme boundary $\mathrm{ex}(\mathcal{G})$, contain more than one element. So far, for models like (2) there exists only one way of establishing the latter fact. Namely, one shows the existence of an element of $\mathcal{G}$, which is not extreme (not a pure state). Recall that $\mathrm{ex}(\mathcal{G})$ is a subset of $\mathcal{G}$. A candidate to be such an element is the so called 'periodic state' which one obtains as the limit of the measures (44) as $L \to +\infty$. For $h = 0$ and big enough β, this state can be *nonergodic* with respect to the translations of $\mathbb{Z}^d$, whereas extreme states are always ergodic. We use this argument in the next section. However, this way essentially employs the $O(\nu)$-symmetry, and hence does not cover case (iii). Therefore, to mathematically describe phase transitions in a wider class of models one needs other definitions, consistent with the physical point of view on this subject. In this subsection, we present and analyze such alternative definitions.

The first definition is based on the celebrated L. D. Landau classification, which employs the differentiability of the free energy density in h, see, e.g., Chapter I in (Bruce and Cowley, 1981). Of course, this property depends also on the value of β. Namely, we say that the model (2) has a *first-order* phase transition at certain values of β and h_*

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[2] Such a statement holds true for the Ising model, see Theorem III.3.11, page 260 in (Simon, 1993), as well as for the model of a nonideal gas in $\mathbb{R}^d$, see (Klein and Wei-Shih Yang, 1993).

if at this β, the polarization $M(h)$ is discontinuous at h_*. The model has a *second-order* phase transition at β and h_* if the first derivative $F'(h)$ is continuous, but the second derivative $F''(h)$ is discontinuous at h_*. Note that these definitions can be applied to version (iii) of our model.

The second definition employs an *order parameter*. It can be applied to cases (i) and (ii) of the model (2) with $h = 0$, which we suppose to be $O(\nu)$-symmetric. One can show that the local states (32) and (33) are such that $\varrho_\Lambda(|q_x|^2)$ and $\varrho_L(|q_x|^2)$ exist and are finite, in spite of the fact that $|q_x|^2$ is an unbounded operator. Then we can consider the Matsubara function, cf. (37) and (43),

$$\Gamma_{xy}^L(\tau, \tau') \tag{61}$$

$$= \frac{1}{Z_L} \sum_{j=1}^\nu \text{trace}\left[q_x^{(j)} e^{-(\tau'-\tau)H_L} q_y^{(j)} e^{-(\beta+\tau-\tau')H_L} \right].$$

Here $0 \leq \tau \leq \tau' \leq \beta$, x and y are points in the cube Λ_L, $L \in \mathbb{N}$, and H_L and Z_L are given in (30) and (31), respectively. According to (38) we have

$$\Gamma_{xy}^L(\tau, \tau') = \sum_{j=1}^\nu \int_{\Omega_{\Lambda_L}} \omega_x^{(j)}(\tau)\omega_y^{(j)}(\tau')\nu_L(d\omega_{\Lambda_L}), \tag{62}$$

where ν_L is given in (44). By the Cauchy-Schwarz inequality, and then by a property of the integrals with respect to ν_L, it follows that

$$\left| \Gamma_{xy}^L(\tau, \tau') \right| \leq \varrho_L(|q_x|^2) \leq C. \tag{63}$$

Note that $\varrho_L(|q_x|^2)$ is independent of x. The meaning of the second inequality in (63) is that the bound C is independent of Λ_L.

As a function of τ and τ', Γ_{xy}^L in (62) can clearly be extended to all values of $(\tau, \tau') \in [0, \beta]^2$. This extension is a continuous function of

$$|\tau - \tau'|_\beta := \min\{|\tau - \tau'|; \beta - |\tau - \tau'|\}.$$

Then the following integral makes sense

$$D_{xy}^L = \beta^{-1} \int_0^\beta \int_0^\beta \Gamma_{xy}^L(\tau, \tau')d\tau d\tau'. \tag{64}$$

If the model (2) is $O(\nu)$-symmetric, as it is in cases (i) and (ii) with $h = 0$, D_{xy}^L describes static correlations between the oscillators located at x and y. In view of the translation symmetry of ν_L, D_{xy}^L is a function of the periodic distance $|x - y|_L$, see (29). Now we introduce, cf. (62),

$$P_L = \frac{1}{\beta|\Lambda_L|^2} \sum_{x,y \in \Lambda_L} D_{xy}^L \tag{65}$$

$$= \int_{\Omega_{\Lambda_L}} \left| \frac{1}{\beta|\Lambda_L|} \sum_{j=1}^\nu \sum_{x \in \Lambda_L} \int_0^\beta \omega_x^{(j)}(\tau)d\tau \right|^2 \nu_L(d\omega_{\Lambda_L}).$$

If D_{xy}^L decays sufficiently fast as $|x - y|_L \to +\infty$, then the double sum in the first line of (65) is of order strictly less than $|\Lambda_L|^2$, and hence $P_L \to 0$ as $L \to +\infty$. On the other hand, by means of (63) we readily obtain that $P_L \leq C$, which means that the sequence $\{P_L\}_{L \in \mathbb{N}}$ is bounded and hence contains convergent subsequences. The largest limit of such subsequences, i.e.,

$$P = \limsup_{L \to +\infty} P_L, \tag{66}$$

is called *order parameter*. We say that, at a given value of β, there exists a *long range order,* if $P > 0$ for this β. In this case, we also say that the model is in an *ordered state*. Thus, we have the following three definitions of a phase transition:

(a) employing thermodynamic phases: $|\text{ex}(\mathcal{G})| > 1$;

(b) employing the polarization jump:
$$M_+(h) \neq M_-(h);$$

(c) employing the order parameter: $P > 0$.

The connections between these notions will be analyzed in the next section.

F. Infrared bounds

The fact that D_{xy}^L is a function of the periodic distance (29) allows us to use the Fourier transformation in the torus Λ_L. Let Λ_L^* denote the Brillouin zone for Λ_L, that is, the set consisting of $p = (p_1, \ldots p_d)$ such that

$$p_i = -\pi + \pi s_i/L, \quad s_i = 1, 2, \ldots, 2L, \quad i = 1, \ldots, d.$$

By $(-\pi, \pi]^d$ we denote the set

$$\{p = (p_1, \ldots, p_d) : p_i \in (-\pi, \pi]\},$$

which is the Brillouin zone for the whole crystal. For $p \in (-\pi, \pi]^d$, we define

$$\widehat{D}_p^L = \sum_{y \in \Lambda_L} D_{xy}^L \exp(\mathrm{i}(p, x - y)). \tag{67}$$

The latter sum is finite for finite L, but can be divergent in the limit $L \to +\infty$. Traditionally, this is called the *infrared divergence*. The restriction of $\widehat{D}_p^L$ to Λ_L^* can be used to define the inverse transform

$$D_{xy}^L = \frac{1}{|\Lambda_L|} \sum_{p \in \Lambda_L^*} \widehat{D}_p^L \exp(-\mathrm{i}(p, x - y))$$

$$= \frac{1}{|\Lambda_L|} \sum_{p \in \Lambda_L^*} \widehat{D}_p^L \cos(p, x - y).$$

Suppose now that we are given a continuous function $\widehat{B} : (-\pi, \pi]^d \to (0, +\infty]$ with the following properties:

$$(a) \quad \int_{(-\pi, \pi]^d} \widehat{B}(p) dp < +\infty; \tag{68}$$

$$(b) \quad \widehat{D}_p^L \leq \widehat{B}(p), \qquad \text{for all } p \neq 0.$$

Since $\widehat{B}$ is independent of L, by (b) one can control the infrared divergence mentioned above. That is why (b) is called an *infrared bound*, see (Kondratiev and Kozitsky, 2006) for more detail on this item. In view of (a), for $x, y \in \mathbb{Z}^d$ the following quantity

$$B_{xy} = \frac{1}{(2\pi)^d} \int_{(-\pi, \pi]^d} \widehat{B}(p) \cos(p, x - y) dp \tag{69}$$

is well-defined. For $x, y \in \Lambda_L$, we also set

$$B_{xy}^L = \frac{1}{|\Lambda_L|} \sum_{p \in \Lambda_L^*, \; p \neq 0} \widehat{B}(p) \cos(p, x - y),$$

and $B_{xy}^L = 0$ if either of x, y belongs to Λ_L^c. One can prove, see Proposition 6.1.2 on page 284 in (Albeverio *et al.*, 2009), that, for every x and y, $B_{xy}^L \to B_{xy}$ as $L \to +\infty$. Furthermore, see Lemma 6.1.3 *ibid*, for every Λ_L and any $x, y \in \Lambda_L$, under the conditions in (68) the following holds

$$D_{xy}^L \geq \left(D_{xx}^L - B_{xx}^L\right) + B_{xy}^L. \tag{70}$$

Note that both D_{xx}^L and B_{xx}^L are independent of x. The meaning of (70) is that the infrared bound (b) in (68) allows one to control from below the decay of the static correlations. Suppose now that there exists a positive ϑ such that, for any cube Λ_L,

$$D_{xx}^L \geq \vartheta. \tag{71}$$

Suppose also that (68) holds and that B_{xy} obeys the following conditions:

$$\text{(a)} \quad \vartheta > B_{xx}; \tag{72}$$

$$\text{(b)} \quad \lim_{|x-y| \to +\infty} B_{xy} = 0.$$

If this is the case, for some $\varepsilon > 0$, all Λ_L and all $x, y \in \Lambda_L$ such that $|x - y| \geq \delta(\varepsilon)$, by (70) we get that $D_{xy}^L \geq \varepsilon$, which yields in (65) that $P_L \geq \varepsilon/\beta$ and hence $P > 0$, see (66). Thus, (71) and (72) imply the existence of the long range order mentioned above.

It turns out that, for our model (2) with any value of the dimension $\nu \in \mathbb{N}$, and with any V, the function $\widehat{B}(p)$ can be found explicitly. The only conditions are that the lattice dimension d should be at least 3 and the interaction in (2) should be of nearest neighbor type, i.e., $J_{xy} = J > 0$ whenever $|x - y| = 1$, and $J_{xy} = 0$ otherwise. Then this function has the following form, see Corollary 6.2.9, page 303 in (Albeverio *et al.*, 2009),

$$\widehat{B}(p) = \frac{\nu}{2J\varepsilon(p)}, \tag{73}$$

$$\varepsilon(p) := \sum_{i=1}^{d} (1 - \cos p_i).$$

Note that $\widehat{B}(p) \sim C|p|^{-2}$, as $|p| \to 0$. Hence, it satisfies condition (a) in (68) only for $d \geq 3$. By (69), we get

$$B_{xx} = \nu\theta(d)/2J, \tag{74}$$

$$\theta(d) := \frac{1}{(2\pi)^d} \int_{(-\pi,\pi]^d} \frac{dp}{\varepsilon(p)}.$$

Then, for any $\vartheta > 0$, condition (a) in (72) can be satisfied by taking big enough J. The validity of (b) in (72) follows by the Riemann-Lebesgue lemma, see Proposition 6.2.10, page 303 in (Albeverio *et al.*, 2009).

III. THE RESULTS

A. Phase transitions

In the first subsection below, we analyze the relationships between the three definitions of a phase transition given above, and then present the corresponding sufficient conditions for the particular versions of our model.

1. The order parameter and the first-order phase transition

First of all we note that the order parameter (66) can be defined without using any path integrals, see (61), (64), and (65). The same is true for the free energy density (53) since

$$F_L(h) = \frac{1}{\beta|\Lambda_L|} \left(\ln Z_L^{\text{har}} - \ln Z_L \right),$$

see (50), (48), and (31). However, the path integral representation of these quantities allows us to apply here measure-theoretic tools, which proved to be useful in classical statistical physics. Namely, by means of Griffiths' theorem, see Theorem 6.1.7, page 286 in (Albeverio *et al.*, 2009), we obtain the following result.

Theorem 2 *Let the dimension ν be arbitrary and the potential V be $O(\nu)$-symmetric and such that the estimate (16) holds. Then the one-sided derivative $M_+(0)$, see (58), and the order parameter P, see (66), obey the estimate*

$$M_+(0) \geq \sqrt{P}. \tag{75}$$

Hence, if the model with such V is in an ordered state, then it undergoes a first-order phase transition.

Indeed, by the assumed symmetry we have $M_+(0) = -M_-(0)$. Hence, $P > 0$ by (75) yields $M_+(0) > 0$, and then $M_-(0) < 0$. Note, however, that the positivity of the order parameter need not yet mean that the thermodynamic phases are multiple. To prove that this is the case we have to impose further restrictions on ν and V.

2. Phase transition in the $|q|^4$ case

Here we suppose that ν is arbitrary and V is as in (13). Recall that $a > 0$ is the rigidity parameter, see (6). Then, for α and b as in (13), we set

$$\vartheta_* = \frac{\nu \alpha}{2b(\nu + 2)}. \tag{76}$$

Note that $\vartheta_* > 0$ whenever $\alpha > 0$ and thereby the potential energy in (6) has multiple minima. For $\nu = 1$, $V(q)$ has two minima at $\pm q_*$, with $q_* = \sqrt{3\vartheta_*}$, cf. (1).

Let $f : [0, +\infty) \to (0, 1]$ be defined as

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

Then, for a fixed $\gamma > 0$, the function

$$\phi(t) := t \gamma f(t/\gamma), \quad t > 0 \tag{77}$$

is differentiable and monotone increasing to γ^2 as $t \to +\infty$, that readily follows from the definition of f. Thus, we set $\gamma = 4m\vartheta_*$ and obtain that the function

$$\frac{1}{2m} J \phi(\beta) = 2\beta J \vartheta_* f(\beta/4m\vartheta)$$

increases as $\beta \to +\infty$ and tends to $8m\vartheta_*^2 J$. Therefore, if the following condition holds

$$8m\vartheta_*^2 J > \theta(d), \tag{78}$$

then the equation

$$2\beta J \vartheta_* f(\beta/4m\vartheta_*) = \theta(d). \tag{79}$$

has a unique solution, which we denote by β_*. The following statement, see Theorem 6.3.6, page 308 in (Albeverio *et al.*, 2009), gives a sufficient condition for a phase transition to occur.

Theorem 3 *Let $d \geq 3$, the interaction intensity be $J_{xy} = J > 0$ whenever $|x - y| = 1$, and $J_{xy} = 0$ otherwise, and let V be as in (13). Suppose also that the condition (78) is satisfied, and hence (79) has the solution β_*. Then, for $\beta > \beta_*$, the following holds: (a) $|\mathrm{ex}(\mathcal{G})| > 1$; (b) $P > 0$; (c) $M_+(0) > M_-(0)$.*

The implication $(b) \Rightarrow (c)$ follows by Theorem 2. The proof of (a) and (b) relies on showing that the estimates (71) and (72) hold with B_{xy} as in (73) and (74). First, for the state (33) and the Hamiltonian (30), and for an appropriate operator A, one readily gets that

$$\varrho_L ([A, [H_L, A]]) \geq 0,$$

where $[H_L, A] = H_L A - A H_L$. Applying this formula with $A = p_x^{(j)}$, $x \in \Lambda_L$ and $j = 1, \ldots, \nu$, and taking into account the form of V and the commutation relations (18), we obtain

$$\varrho_L \left(|q_x|^2 \right) \geq \vartheta_*. \tag{80}$$

Next, we employ the Bruch-Falk inequality, see also (Dyson *et al.*, 1978) and page 392 in (Simon, 1993), and obtain from the latter that

$$D_{xx}^L \geq \beta \nu \vartheta_* f \left(\frac{\beta}{4m\vartheta_*} \right), \tag{81}$$

where f is as in (77). This estimate and (74) yield

$$D_{xx}^L - B_{xx} \geq \beta \nu \vartheta_* f \left(\frac{\beta}{4m\vartheta_*} \right) - \frac{\nu \theta(d)}{2J}. \tag{82}$$

For $\beta > \beta_*$, the right-hand side of (82) is strictly positive. Then D_{xy}^L does not decay to zero as $L \to +\infty$ and $|x - y|_L \to +\infty$. This yields $P > 0$, see (65). This also yields that the periodic state is not ergodic with respect to the group of translations of $\mathbb{Z}^d$, implying that $\mathcal{G}$ contains elements which do not belong to $\mathrm{ex}(\mathcal{G})$, see Definition 3.1.26 and Corollary 3.1.29, page 207 in (Albeverio *et al.*, 2009). By this we get that $|\mathcal{G}| > 1$, which proves also *(a)*.

3. Phase transition in the $\nu = 1$ symmetric case

Here we assume that $V(q) = V(-q)$ and (14) is satisfied. In addition, we assume that there exists $J > 0$ such that, for all $x, y \in \mathbb{Z}^d$ obeying $|x - y| = 1$, the following holds

$$J_{xy} \geq J. \tag{83}$$

Let Φ be as in (17). Then the equation

$$-2b_1 + \Phi(\vartheta) = 0, \tag{84}$$

has a unique solution $\vartheta_* > 0$, since $b_1 > 0$, see (15). In this case, we have the following result, see Theorem 6.3.8, page 310 in (Albeverio *et al.*, 2009).

Theorem 4 *Let the model be as just described and let the condition in (78) be satisfied with ϑ_* defined by (84) and J obeying (83). Then, for every $\beta > \beta_*$ defined by (79), the following holds: (a) $|\mathrm{ex}(\mathcal{G})| > 1$; (b) $P > 0$; (c) $M_+(0) > M_-(0)$.*

Again, as above (b) implies (c) by Theorem 2. Claims (a) and (b) are proven by comparing the considered model with the model described by the Hamiltonian

$$H^{\mathrm{low}} = -\frac{J}{2} \sum_{x,y:\ |x-y|=1} q_x q_y + \sum_x \left[\frac{1}{2m} p_x^2 + W(q_x) \right], \tag{85}$$

where W is as in (15). Then we use the GKS inequalities, which hold in the considered case, see Theorem 2.2.2, page 163 in (Albeverio *et al.*, 2009), and a comparison method developed in (Kozitsky and Pasurek, 2007). By means of these tools we prove that if (a) and (b) hold for the model as in (85), they hold also for that of (2) with such V and $\nu = 1$. On the other hand, the properties of W allow us to prove that (81) holds for the model (85) with ϑ_* defined by (84). The infrared bound (67) with $\widehat{B}_p$ as in (73) also holds since the interaction is of nearest-neighbor type. Then the proof of (a) and (b) for the model (85) follows as for Theorem 3.

4. Phase transition in the $\nu = 1$ asymmetric case

In case (iii) of the model (2), the only result concerning phase transitions which we managed to get so far is a statement that the model parameters and the inverse temperature β can be chosen in such a way that the polarization $M(h)$ becomes discontinuous at certain h_*, i.e., the model has a first-order phase transition, see Theorem 3.4 of (Kargol *et al.*, 2008) and Section 6.3.3 of (Albeverio *et al.*, 2009).

Theorem 5 *Suppose that $\nu = 1$, $d \geq 3$, the interaction is of nearest-neighbor type, and V is continuous and such that (16) holds, which includes the case of $V(q) \neq V(-q)$. Then, for every $\beta > 0$, there exist $m_* > 0$ and $J_* > 0$ such that, for all $m > m_*$ and $J > J_*$, there exists $h_* \in \mathbb{R}$, possibly dependent on m, β, and J, such that the polarization $M(h)$ becomes discontinuous at $h = h_*$, i.e., the model has a first-order phase transition.*

Here we again exploit the fact, used in the proof of Theorem 3, that the existence of a nonergodic state implies $|\mathcal{G}| = +\infty$, and hence a first-order phase transition. Recall that the existence of a nonergodic periodic state would follow from the fact that the static correlation function $D_{xy}^L - [M_L(h)]^2$ does not decay to zero as $L \to +\infty$ and $|x - y|_L \to +\infty$. The latter means that there exists a sequence of integer numbers $\{L_n\}_{n \in \mathbb{N}}$ such that $L_n \to +\infty$ and the following holds

$$D_{xy}^{L_n} - [M_{L_n}(h)]^2 \geq \delta, \tag{86}$$

for some $\delta > 0$, all x, y, and all n such that $x, y \in \Lambda_{L_n}$. Note that in the symmetric case, we have $M_L(0) = 0$, and hence (70) can be used. Suppose now that there exists h_0 such that $M(h_0) = 0$. Since $M(h_0) = \lim M_L(h_0)$, see (60), for such h_0 (86) would follow from the fact that

$$D_{xy}^{L_n} \geq \delta. \tag{87}$$

Thus, if (87) holds and $M(h)$ takes both negative and positive values, then either $M(h_0) = 0$, and thus (86) yields a first-order phase transition, or $M(h)$ is discontinuous, which yields the same.

To realize this scheme we crucially use the properties of our path integrals. As was mentioned above, the free energy density $F(h)$ is a concave function of $h \in \mathbb{R}$, see (57). Then the set of such h where $M_+(h) \neq M_-(h)$, and hence $M(h)$ does not exist, is at most countable. Let $\mathcal{R}$ denote the set of all $h \in \mathbb{R}$ for which $M(h)$ exists. Then any interval $(a, b) \subset \mathbb{R}$ contains points of $\mathcal{R}$. A tedious analysis of the properties of the path integrals used in our constructions yields the following estimate of the free energy density (50)

$$-F_L(h) \geq h\varepsilon + \Psi(\beta) + \Xi(m), \tag{88}$$

see Theorem 5.2.2, page 271 in (Albeverio *et al.*, 2009). This estimate holds for all $h \geq 0$, $J \geq 0$, and $m > m_0$, where $m_0 > 0$ is a certain quantity which may depend on β. Here $\varepsilon > 0$ is a constant, and Ψ and Ξ are certain real-valued continuous functions of β and m, which can be calculated explicitly. As the right-hand side of (88) is independent of L, this estimate holds also in the limit $L \to +\infty$, for all h such that $M(h)$ exists. By the mentioned concavity of $F(h)$, for any such $h \geq 0$, we have

$$M(h) \geq [F(0) - F(h)]/h$$

$$\geq \varepsilon + [F(0) + \Psi(\beta) + \Xi(m)]/h.$$

Since the right-hand side of the latter inequality tends to $\varepsilon > 0$ as $h \to +\infty$, $M(h)$ becomes positive for big enough h. Thus, there exists $h_+ > 0$ such that $M(h) > 0$ for all $h \in \mathcal{R} \cap (h_+, +\infty)$. Likewise, one can show that there exists $h_- < 0$ such that $M(h) < 0$ for all $h \in \mathcal{R} \cap (-\infty, h_-)$. Next, some additional analysis of the path integral in the representation

$$\varrho_L\left(q_x^2\right) = \int_{\Omega_{\Lambda_L}} [\omega_x(0)]^2 \, \nu_L(d\omega_{\Lambda_L}),$$

cf. (44), yields, see Lemma 6.3.9, page 312 in (Albeverio *et al.*, 2009), that, for every positive β and ϑ_*, there exist positive m_1 and J_*, which may depend on β and ϑ_* but are independent of h, such that, for any cube Λ_L and any $h \in \mathbb{R}$, and for all $J > J_*$ and $m > m_1$, the following holds

$$\varrho_L\left(q_x^2\right) \geq \vartheta_*. \tag{89}$$

Then the proof of Theorem 5 follows along the next line of arguments. Fix any ϑ_* and take $m > m_* := \max\{m_0; m_1\}$. Then both (88) and (89) hold. Hence, in view of (89), we have that (81) and (82) hold for such β and m, and for all L and h. Then we increase J, if necessary, up to the value at which the right-hand side of (82) gets strictly positive. Afterwards, all the parameters, except for h, are kept fixed. By (70), the positivity of the RHS of (82) yields (87). If $M(h)$ were everywhere continuous, the fact that it takes both positive and negative values would imply that there exists h_0 such that $M(h_0) = 0$, which together with (87) would yield (86). The latter, however, contradicts the everywhere continuity of M, see Theorem 1.

B. Quantum effects

1. The stability of quantum crystals

To understand what makes a crystal stable or unstable let us first consider the scalar ($\nu = 1$) harmonic version of the model (2), in which $H_x = H_x^{\text{har}}$, see (6). For this model, the global Gibbs states, and hence the thermodynamic phases as mathematical objects, can be constructed only if the stability condition

$$\hat{J}_0 < a = m[\Delta^{\text{har}}]^2$$

is satisfied, see (5) and (20). In this case, $|\mathcal{G}| = 1$ for all β, see also Theorem 6 below . If $\hat{J}_0 = a$, the harmonic crystal becomes unstable with respect to spatial translations; for $d \geq 3$, the set $\mathcal{G}$ is still a singleton, and $\mathcal{G} = \emptyset$ for $d \leq 2$, because of the divergence of integrals as in (74) for such values of d. In the anharmonic case, due to the assumption (16) global Gibbs states exist for all $\hat{J}_0 > 0$, and the instability of the crystal can be caused by the 'effective' change of the equilibrium positions of oscillators, i.e., by a structural phase transition. Thus, according to Theorem 2, a sufficient condition for a d-dimensional quantum crystal, $d \geq 3$, to have multiple thermodynamic phases at a given β is

$$\beta \hat{J}_0 \vartheta_* f\left(\frac{\beta}{4m\vartheta_*}\right) > d\theta(d), \tag{90}$$

which in the classical limit $m \to +\infty$, cf. (9), takes the form

$$\beta \hat{J}_0 \vartheta_* > d\theta(d).$$

The latter condition can be satisfied by picking big enough β. Therefore, the classical anharmonic crystal with $d \geq 3$ always has a phase transition - no matter how small $\hat{J}_0$ is. For finite m, the left-hand side of (90) is bounded by $4m\vartheta_*^2 \hat{J}_0$, and the bound is achieved in the limit $\beta \to +\infty$. Thus, if

$$Q := 4m\vartheta_*^2 \hat{J}_0 \leq d\theta(d), \tag{91}$$

the condition (90) will not be satisfied for any $\beta > 0$. Although (90) is only a sufficient condition, one might expect that the phase transition cannot occur at any β if the parameter Q is small. This effect could be called *quantum stabilization*. The following statement shows that this really occurs.

Theorem 6 *Let $\nu = 1$ and the potential V be as in (19). Then the set $\mathcal{G}$ of the Gibbs states of the corresponding model is a singleton at all $\beta > 0$ under the following condition*

$$\hat{J}_0 < R_m. \tag{92}$$

Thus, in this case there is no phase transitions at all temperatures.

This statement is an adaptation of Theorem 7.3.1, page 346 in (Albeverio *et al.*, 2009). Thus, (92) is the condition under which the mentioned quantum stabilization holds. In view of (26), it can be satisfied by picking small enough m.

To relate (92) with (91), we use the following result, see Theorem 7.1.1, page 338 in (Albeverio *et al.*, 2009).

Theorem 7 *Let ν and V be as in Theorem 6. Then the rigidity parameter obeys the estimate*

$$R_m \leq \frac{1}{4m\vartheta_*^2}. \tag{93}$$

This estimate clearly shows that R_m describes the tunneling motion between the wells. For if ϑ_* is big, cf. (76), then R_m gets small. On the other hand, for small ϑ_*, the bound (93) becomes inessential, and hence R_m can be arbitrary. For such ϑ_*, we lose the control of R_m. This includes the case of convex V where $\vartheta_* = 0$, as it is for harmonic crystals.

Thus, if (92) holds, then

$$Q < \varkappa := 4m\vartheta_*^2 R_m \leq 1. \tag{94}$$

It is known, cf. Proposition 6.3.5, page 308 in (Albeverio *et al.*, 2009), that $d\theta(d) > 1$, and

$$\frac{1}{d - 1/2} < \theta(d) < \frac{1}{d - 1}, \tag{95}$$

for $d \geq 4$. Therefore, for the phase transition to be suppressed at all temperatures, it suffices that (94) holds, whereas (91) is the corresponding necessary condition. By (95), the right-hand side of (91) is close to one for big d. Thus, for such d the gap between these two conditions is close to $1 - \varkappa$.

2. Normality of fluctuations in the $\nu > 1$ case

Unfortunately, we cannot extend Theorem 6 to the vector case $\nu > 1$. The main reason for this is that the eigenvalues of the corresponding H_x are no longer simple. The only result of this kind which so far we can get is that the fluctuations of the displacements q_x remain normal at all temperatures under a condition similar to (92).

Here we again suppose that the potential V is $O(\nu)$-symmetric. Then the operator which describes fluctuations of the displacements of oscillators in a given Λ is

$$F_{j,\Lambda}^{(\sigma)} = \frac{1}{|\Lambda|^{\sigma/2}} \sum_{x \in \Lambda} q_x^{(j)}, \quad j = 1, \ldots, \nu, \quad \sigma \geq 1. \tag{96}$$

Let us introduce the following parameter

$$P_\Lambda^{(\sigma)} = \frac{1}{\beta} \sum_{j=1}^{\nu} \int_0^\beta \int_0^\beta \Gamma_{F_{j,\Lambda}^{(\sigma)} F_{j,\Lambda}^{(\sigma)}}(\tau, \tau') d\tau d\tau'.$$

Then $P_L = P_{\Lambda_L}^{(2)}$, cf. (65). Clearly, if $P > 0$, then $P_{\Lambda_L}^{(\sigma)} \to +\infty$ as $L \to +\infty$, for any $\sigma \in [1, 2)$. We say that the fluctuations of the displacements of oscillators are *normal* if the Matsubara functions (37) for the operators (96) with $\sigma = 1$ remain bounded as $\Lambda \to \mathbb{Z}^d$.

Since V is $O(\nu)$-symmetric, there exists $v(t)$, $t \geq 0$, such that $V(q) = v(|q|^2)$. Let Δ be the gap parameter (21) of the Hamiltonian

$$\widetilde{H}_x := \frac{1}{2m} p_x^2 + v(q_x^2), \tag{97}$$

of a one-dimensional oscillator with the same m as the considered ν-dimensional oscillator. The following result is an adaptation of Theorem 7.3.5, page 350 in (Albeverio *et al.*, 2009).

Theorem 8 *Let $\nu > 1$ be arbitrary, V obey (16), and let the condition (92) be satisfied in which Δ is the gap parameter (21) of the Hamiltonian (97). Then the fluctuations of the displacements of oscillators in the corresponding model remain normal at all temperatures.*

The proof of this result relies on the so called scalar domination estimates obtained in Theorem 2.5.2, page 175 of (Albeverio *et al.*, 2009), see also (Kozitsky, 2000b).

3. Decay of correlations

For simplicity, we suppose here that the model (2) is of type (i), cf. (13), with $\nu = 1$. For this model, the Matsubara function (62) describes the displacement-displacement correlations in the local periodic state (33). In the limit $L \to +\infty$, we obtain periodic Gibbs states, possibly multiple. Under the stability condition (92), there is only one such state. Then we set

$$\Gamma_{xy}(\tau, \tau') = \lim_{L \to +\infty} \Gamma_{xy}^L(\tau, \tau'). \tag{98}$$

We know that $\Gamma_{xy}(\tau, \tau')$ should vanish in the limit $|x - y| \to \infty$, otherwise the corresponding state would be nonergodic. The following statement, which is an adaptation of Theorem 7.2.2, page 344 in (Albeverio *et al.*, 2009), describes the spatial decay of (98).

Theorem 9 *Let the stability condition (92) be satisfied. Then the correlation function (98) has the bound*

$$\Gamma_{xy}(\tau, \tau') \leq \frac{1}{\beta(2\pi)^d} \sum_{k \in \mathcal{K}} \int_{(-\pi,\pi]^d} \frac{\exp\left[\mathrm{i}(p, x - y) + \mathrm{i}k(\tau - \tau')\right]}{m(\Delta^2 + k^2) + \Upsilon(p)} dp, \tag{99}$$

where

$$\Upsilon(p) = 2 \sum_y J_{xy} \left[\sin(p, x - y)\right]^2,$$

and $\mathcal{K}$ is the set of all $k = (2\pi/\beta)\kappa$, $\kappa \in \mathbb{Z}$.

One observes that the right-hand side of (99) is the correlation function of a quantum harmonic crystal with the single-oscillator rigidity $m\Delta^2$. Thus, under the condition (92) the decay of (98) is at least as strong as it is in the corresponding stable quantum harmonic crystal. This result is valid for arbitrary J_{xy} obeying (5). If the interaction has finite range, then $\Upsilon(p) \sim C|p|^2$ for some $C > 0$. In this case, the spatial decay of the right-hand side of (99), and hence of $\Gamma_{xy}(\tau, \tau')$, is exponential, see Theorem 7.2.4, page 345 in (Albeverio *et al.*, 2009).

IV. CONCLUDING REMARKS

A. To Section II

1. The model

In ionic crystals, the ions usually form massive complexes which determine the physical properties of the crystal, including the instability with respect to structural phase transitions. Such massive complexes can be considered as classical particles which obey the rules of classical statistical mechanics. At the same time, in a number of ionic crystals certain aspects of the phase transitions are apparently unusual from the point of view of classical physics, and can be explained only in a quantum-mechanical context. Such crystals contain light localized ions, and thus the mentioned features of their behavior point to the essential role of these light ions. In the simplest models of these crystals the motion of heavy complexes is ignored – their only role is to create a potential field for the light particles. In this case, the relevant model parameters are those which describe this field, the masses of the light particles, and the interaction strength. Therefore, a consistent theory of phase transitions in such models should describe the influence of all these parameters. We refer the reader to the survey article (Stamenković, 1998) for more detailed arguments in favor of the model given in (2).

The mathematical theory of a harmonic oscillator is quite standard, its updated and detailed presentation can be found in (Albeverio *et al.*, 2009), pages 36–44. The theory of an anharmonic oscillator with a convex potential energy is also quite standard. For instance, the case of $H_x = H_x^{\mathrm{har}} + bq^{2r}$, $b > 0$ and $r \geq 2$, was carefully analyzed in (Banerjee, 1978). However, convex potentials do not have multiple wells, whereas the tunneling between the wells is the basic phenomenon in the studied substances. The theory outlined above in subsection II.B among others employs quite recent results on Schrödinger operators obtained in (Auscher and Ben Ali, 2007). By means of them we found out for which potentials V the domain of self-adjointness of H_x can be established exactly. This in turn allowed us to study the gap parameter (21) in great detail. Quite often, see, e.g., (Ankerhold , 2007) and (Combes *et al.*, 1983), the description of the tunneling between the wells is concentrated on semiclassical expansions for the gap parameter $E_1 - E_0$, which in our case would be in negative powers of $m = m_{\mathrm{ph}}/\hbar^2$. Our analysis is essentially different, since it covers the case of 'strong quantum effects' where semiclassical arguments are not applicable.

2. Thermodynamic phases and the free energy

The use of thermodynamic phases as mathematical objects is crucial in the rigorous description of thermodynamic properties of a given model. In classical equilibrium statistical physics, see (Georgii, 1988), (Simon, 1993), and (Sinai , 1982), thermodynamic phases appear as extreme elements of the set of Gibbs measures. For quantum models described by bounded Hamiltonians, thermodynamic phases are pure KMS states, i.e., positive normalized linear functionals on algebras of quasi-local observables which obey the Kubo-Martin-Schwinger conditions, see Section 6.2 in (Bratteli and Robinson, 1981). However, for quantum anharmonic crystals described by unbounded Hamiltonians, the direct construction of such KMS states appears to be impossible, see, e.g., the discussion in (Inoue, 2000). In this situation, the construction of thermodynamic phases as path measures realized in (Albeverio *et al.*, 2009) seems to be the only possible way to settle the problem. It is performed by means of local Gibbs measures, cf. (39), within the general scheme developed in (Georgii, 1988). The most significant point of our technique is the representation of Matsubara functions in the form of path integrals, see (38). The local Gibbs measure ν_Λ (39) which appears in this representation is constructed from the corresponding Hamiltonian (27). The harmonic part $\sum_{x \in \Lambda} H_x^{\mathrm{har}}$ of the latter is represented in (39) by the measure χ_Λ (42), which is the Gibbs measure of noninteracting harmonic oscillators located in Λ. The interaction, the anharmonic part of H_Λ, as well as the external field term are taken into account in the energy functional (40). By means of a technique developed in Chapter 2 of (Albeverio *et al.*, 2009) the measure (39) is approximated by the Gibbs measure of a system of classical ν-dimensional oscillators living on a $d+1$-dimensional lattice, see Section 2.1 *ibid*. This extra dimension appears, in particular, when one approximates the integrals in (40) by finite sums. Thus, the key feature of our method of studying thermodynamic states of the model (2) is that we describe it as a system of classical oscillators performing 'infinite dimensional oscillations'.

The most significant fact about the free energy density is its universality expressed in the equality (54). A deep fact behind it is the existence of van Hove sequences of subsets of $\mathbb{Z}^d$. It is known that such sequences do not exist for non-amenable graphs, e.g., for a Bethe lattice. In this case, the phase diagram of an Ising model is completely different, compared to that of this model on $\mathbb{Z}^d$. In particular, phase transitions can occur at nonzero h, cf. Theorem 1 above and (Lyons, 2000). The mentioned universality, as well as the concavity of $F(h)$ which follows from the

property (57), allow one to get the polarization (59), and hence to study phase transitions.

3. Phase transitions, order parameters, and infrared bounds

When one deals with thermodynamic phases, the most general definition of a phase transition is the multiplicity of such phases existing at the same values of the model parameters and of the temperature and an external field, see Chapter 7 in (Georgii, 1988). Another possibility to define a phase transition, which goes back to L. D. Landau, is to use the differentiability property of the free energy density $F(h)$ as a function of the external field h. One more possibility is to employ an order parameter, cf. (65) and (66). For an Ising model, all the three definitions are equivalent, see (Simon, 1993). In our case, however, we managed to establish only the fact stated in Theorem 2. For versions of the model (2), phase transitions were previously discussed mostly by means of the order parameter, see (Minlos *et al.*, 2002; Schneider *et al.*, 1976; Stamenković *et al.*, 1987; Verbeure and Zagrebnov, 1993, 1995). The reason for this is that, in such a case, one needs to control the Matsubara functions (63) only, which can be done not only by path measures.

The way of establishing phase transitions in quantum lattice models by means of infrared estimates was suggested in (Dyson *et al.*, 1978). To the model (2), in the present form it was developed in (Kargol *et al.*, 2008). The key idea of this method is to show that the spatial correlations do not decay to zero at large distances. This would point to the existence of a Gibbs state which is not ergodic with respect to the lattice translations, and hence to the multiplicity of thermodynamic phases. The key point here is the estimate in (70), where the first summand in the lower bound of D_{xy}^L is independent of x. Then the property in question is obtained if (72) is satisfied.

B. To Section III:

1. Phase transitions

As was mentioned above, in our approach the system of quantum anharmonic oscillators is described as a system of classical oscillators performing 'infinite dimensional oscillations'. This allows us to apply here the original version of the infrared estimates (Fröhlich *et al.*, 1976) adapted to the infinite dimensional case. The most transparent proof of the existence of a phase transition is in the $|q|^4$ case. The way of passing from (80) to the key estimate (81) was suggested in (Dyson *et al.*, 1978) where the function f as in (79) was introduced. The condition (78) is surprisingly simple. In fact, it points to a quantum phase transition which would occur at zero temperature. If (78) holds, then there exist multiple 'ground states' of the model, whereas (94) implies that the 'ground state' is unique. Of course, such a 'ground state' ought to be defined as a mathematical object. For a simpler version of the model (2), this was done in (Albeverio *et al.*, 2000). The extension of Theorem 3 to more general models made in Theorem 4 was done by means of a comparison method elaborated in (Kozitsky and Pasurek, 2007) and based on a tedious analysis of path measures. The result of Theorem 5 was first established in (Kargol *et al.*, 2008). Its main conclusion is that a first order phase transition can occur without symmetry breaking. The way of getting this result was crucially based on the properties of path measures.

2. Quantum effects

As was mentioned above, the first paper where quantum effects in models like (2) were discussed is (Schneider *et al.*, 1976). However, only the systematic use of path measures, which allows for dealing with thermodynamic states as mathematical objects, leads to the most complete description of such effects. Note also that a tedious analysis of the spectral properties of a single anharmonic oscillator was crucial. The first paper where the notion of quantum stabilization was introduced is (Albeverio *et al.*, 2003a). The key parameter is the quantum rigidity (25). When it is large, the oscillator 'forgets' about the details of the potential energy in H_x in the vicinity of the origin (including instability) and oscillates as if its equilibrium were stable, as in the harmonic case. The results of Theorem 8 were obtained in (Kozitsky, 2000a) by means of the so called scalar domination inequalities obtained in (Kozitsky, 2000b). The result of Theorem 9 was obtained in (Kondratiev and Kozitsky, 2003). The first systematic study of phase transitions and quantum effects in the model (2) based on path integral methods was done in (Kargol *et al.*, 2008).

ACKNOWLEDGMENTS

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