Phase Transitions and Quantum Stabilization in Quantum Anharmonic Crystals

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Abstract

A unified theory of phase transitions and quantum e ects in quan-

The quantum crystal studied in this article is a system of interacting quantum anharmonic oscillators indexed by the elements of a crystal lattice L, which for simplicity we assume to be a d-dimensional simple cubic lattice Z^d. The quantum anharmonic oscillator is a mathematical model of a quantum particle moving in a potential field with possibly multiple minima, which has a sufficient growth at infinity and hence localizes the particle. Most of the models of interacting quantum oscillators are related with solids such as ionic crystals containing localized light particles oscillating in the field created by heavy ionic complexes, or quantum crystals consisting entirely of such particles. For instance, a potential field with multiple minima is seen by a helium atom located at the center of the crystal cell in bcc helium, see page 11 in [43]. The same situation exists in other quantum crystals, He, H_2 and to some extent Ne. An example of the ionic crystal with localized quantum particles moving in a double-

where m_{ph} is the physical mass of the particle. Therefore, the commutation relation for the components of the momentum and displacement takes the form

$$p_{\alpha}^{(j)} q_{\alpha'}^{(j')} - q_{\alpha'}^{(j')} p_{\alpha}^{(j)} = -\imath\delta_{\alpha\alpha'}\delta_{jj'}, \quad j, j' = 1, \ldots, \nu. \tag{1.4}$$

For a detailed discussion on how to derive a model like (1.1), (1.2) from physical models of concrete substances, we refer the reader to the sur

strong in the small mass limit, which was in agreement with the experimental data, e.g., on the isotopic e ect in the ferroelectrics with hydrogen bounds, see

2 Euclidean Gibbs States

The main element of the Euclidean approach is the description of the equilibrium thermodynamic properties of the model (1.1), (1.2) by means of Euclidean Gibbs states, which are probability measures on certain configuration spaces. In this section, we briefly describe the main elements of this approach which are then used in the subsequent parts of the article. For more details, we refer to [54].

2.1 Local Gibbs states

Let us begin by specifying the properties of the model described by the Hamiltonian (1.1). The general assumptions regarding the interaction intensities $\mathbf{J}_{\square\square'}$ are

$$\mathbf{J}_{\square\square'} = \mathbf{J}_{\square'\square} \geq 0, \quad \mathbf{J}_{\square\square} = 0, \quad \hat{\mathbf{J}}_0 \stackrel{\text{def}}{=} \sup_{\square} \sum_{\square'} \mathbf{J}_{\square\square'} < \infty$$

where

$$Z_\Lambda = \mathrm{trace}[\exp(-\beta H_\Lambda)] < \infty \tag{2.6}$$

is the partition function, and C_Λ is the algebra of all bounded linear operators on $L^2(R^{\nu|\Lambda|})$. Note that adjective *local* will always stand for a property related with a certain $\Lambda \Subset L$, whereas *global* will characterize the whole infinite system.

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

2.3 Local Euclidean Gibbs measures

Now we construct the measure ν_Λ which appears in (2.15). A single harmonic oscillator is described by the Hamiltonian, c.f., (1.2),

$$\mathsf{H}_{\Lambda}^{\mathrm{har}} = -\frac{1}{2}$$

Proposition 2.2 (Fernique) *For every* $\sigma \in (0, 1/2)$, *there exists* $\lambda_\sigma > 0$, *which can be estimated explicitely, such that*

$$\int_{L^2_\beta} \exp\left[\lambda_\sigma \|\varphi\|^2_{C^\sigma_\beta}\right] \chi(d\varphi) < \infty. \tag{2.29}$$

The second property follows from the estimate (2.27) by the Garsia-Rodemich-Rumsey lemma, see [29]. For fixed $\sigma \in (0, 1/2)$, we set

$$\Xi_\vartheta(\omega) = \sup_{\tau,\tau' :\, 0<|\tau-\tau'|_\beta<\vartheta} |\omega(\tau) - \omega(\tau')|$$

where

$$Z_\Lambda^{\mathrm{har}} \stackrel{\mathrm{def}}{=} \operatorname{trace} \exp\Big[-\beta \sum_{\square \subset \Lambda} H_\square^{\mathrm{har}}\Big] = \Big[\exp\big[-(\beta/2)\sqrt{a/m}\big]\Big]^{\nu|\Lambda|} \Big/ \Big[1-\exp\big[-\beta\sqrt{a/m}\big]\Big] \,.$$

Now let us summarize the connections between the description of the subsystem located in $\Lambda \Subset \mathsf{L}$ in terms of the states (2.5) and of the Euclidean Gibbs measures (2.33). By the density theorem, the state ω_Λ is fully determined by the Green functions (2.8) corresponding to all choices of $n \in \mathbb{N}$ and $F_1, \ldots, F_n \in \mathcal{F}_\Lambda$. Then the multiple-time analyticity theorem leads us from the Green functions to the Matsubara functions (2.12), which then are represented as integrals over path spaces with respect to the local Euclidean Gibbs measures, see (2.15). On the other hand, these integrals taken for all possible choices of bounded continuous functions $F_1, \ldots, F_n$ fully determine the measure ν_Λ. Thereby, we have a one-to-one correspondence between the local Gibbs states (2.5) and the states on the algebras of bounded continuous functions determined by the local

totic properties of J_{xy}, $|x - y| \to +\infty$, see (2.1). If for a certain $\alpha > 0$,

$$\sup_x \sum_y J_{xy} \exp(\alpha|x - y|) < \infty, \tag{2.41}$$

then the weights $\{w_\alpha(x, y)\}_{\alpha \in I}$ are chosen as

$$w_\alpha(x, y) = \exp(-\alpha|x - y|), \qquad I = (0, \bar{\alpha}), \tag{2.42}$$

where $\bar{\alpha}$ is the supremum of $\alpha > 0$, for which (2.41) holds. If the latter condition does not hold for any $\alpha > 0$, we assume that

$$\sup_x \sum_y J_{xy} \cdot (1 + |x - y|)^{\alpha d}, \tag{2.43}$$

for a certain $\alpha > 1$. Then we set $\bar{\alpha}$ to be the supremum of $\alpha > 1$ obeying (2.43) and

$$w_\alpha(x, y) = (1 + \varepsilon|x - y|)^{-\alpha d}, \tag{2.44}$$

where $\varepsilon > 0$ is a technical parameter. In the sequel, we restrict ourselves to these two kinds of J_{xy}. For more details on this item, we refer the reader to [54].

Given $\alpha \in I$ and $\omega \in \Omega$, we set

$$\|\omega\|_\alpha = \left(\sum_x \|\omega_x\|^2_{L^2_\beta} w_\alpha(0, x) \right)^{1/2}, \tag{2.45}$$

and

$$\Omega_\alpha = \{\omega \in \Omega \mid \|\omega\|_\alpha < \infty\}. \tag{2.46}$$

Thereby, we endow Ω_α with the metric

$$\rho_\alpha(\omega, \omega') = \|\omega - \omega'\|_\alpha + \sum_x 2^{-|x|} \frac{\|\omega_x - \omega'_x\|_{C_\beta}}{1 + \|\omega_x - \omega'_x\|_{C_\beta}}, \tag{2.47}$$

which turns it into a Polish space. The set of tempered configurations is defined to be

$$\Omega^t = \bigcap_{\alpha \in I} \Omega_\alpha. \tag{2.48}$$

We endow it with the projective limit topology, which turns it into a Polish space as well. For every $\alpha \in I$, the embeddings $\Omega^t \to \Omega_\alpha \to \Omega$ are continuous; hence, $\Omega_\alpha, \Omega^t \in \mathbf{B}(\Omega)$ and the Borel σ-algebras $\mathbf{B}(\Omega_\alpha)$, $\mathbf{B}(\Omega^t)$ coincide with the ones induced on them by $\mathbf{B}(\Omega)$.

2.5 Local Gibbs specification

Let us turn to the functional (2.38). By standard methods, one proves that, for every $\alpha \in I$, the map $\Omega_\alpha \times \Omega_\alpha \ni (\omega|\xi) \mapsto H_\Lambda(\omega|\xi)$ is continuous. Furthermore,

In view of (2.66), the one-site projections of each $\mu \in \mathcal{G}^{t}$ are sub-Gaussian. The constant C does not depend on Λ and is the same for all $\mu \in \mathcal{G}^{t}$, though it may depend on σ and κ. The estimate (2.66) plays a crucial role in the theory of the set $\mathcal{G}^{t}$.

According to [30] certain Gibbs states correspond to the thermodynamic phases of the underlying physical system. Thus, in our context multiple phases exist only if $\mathcal{G}^{t}$ has more than one element for appropriate values of β and the model parameters. On the other hand, a priori one cannot exclude that this set always has multiple elements, which would make it useless for describing phase transitions. The next statement which we present here[2] clarifies the situation. Let us decompose

$$V_{\Lambda} = V_{1,\Lambda} + V_{2,\Lambda}, \tag{2.67}$$

where $V_{1,\Lambda} \in C^{2}(\mathbb{R}^{\nu})$ is such that

$$-a \le b \stackrel{\text{def}}{=} \inf_{\Lambda} \inf_{x,y \in \mathbb{R}^{\nu},\, y \neq 0} V''_{1,\Lambda}(x)y, y \rangle / |y|^{2} < \infty. \tag{2.68}$$

As for the second term, we set

$$0 \le \delta \stackrel{\text{def}}{=} \sup_{\Lambda} \Big[\sup_{x \in \mathbb{R}^{\nu}} V_{2,\Lambda}(x) - \inf_{x \in \mathbb{R}^{\nu}} V_{2,\Lambda}(x) \Big] \le \infty. \tag{2.69}$$

Its role is to produce multiple minima of the potential energy responsible for eventual phase transitions. Clearly, the decomposition (2.67) is not unique; its optimal realizations for certain types of V_{Λ} are discussed in section 6 of [13]. Recall that the interaction parameter $\hat{J}_0$ was defined in (2.1).

Proposition 2.14 *The set $\mathcal{G}^{t}$ is a singleton if*

$$e^{\beta\delta} < (a + b)/\hat{J}_0. \tag{2.70}$$

Remark 2.15 *The latter condition surely holds at all β if*

$$\delta = 0 \quad \text{and} \quad \hat{J}_0 < a + b. \tag{2.71}$$

If the oscillators are harmonic, $\delta = b = 0$, which yields the stability condition

$$\hat{J}_0 < a. \tag{2.72}$$

The condition (2.70) does not contain the partic

By means of (2.78) we introduce the periodic Hamiltonian

$$H_\Lambda^{\mathrm{per}} = H_\Lambda = -\frac{1}{2}\sum_{\square,\square'\square\Lambda} J^{\Lambda}_{\square\square'}\cdot(q_\square, q_{\square'}) + \sum_{\square\square\Lambda} H_\square, \tag{2.83}$$

and the corresponding periodic local Gibbs state

$$\square^{\mathrm{per}}_\Lambda(A) = \mathrm{trace}[A\exp(-\beta H^{\mathrm{per}}_\Lambda)]/\mathrm{trace}[\exp(-\beta H^{\mathrm{per}}_\Lambda)], \quad A \square C_\Lambda. \tag{2.84}$$

The relationship between the measure $\nu^{\mathrm{per}}_\Lambda$ and this state is the same as in the case of ν_Λ and $\square_\Lambda$.

Set, c.f., (2.50),

$$\pi^{\mathrm{per}}_\Lambda(B) = \frac{1}{N^{\mathrm{per}}_\Lambda}\int_{\Omega_\Lambda} \exp[-I^{\mathrm{per}}_\Lambda(\omega_\Lambda)]\, I_B(\omega_\Lambda \times 0_{\Lambda^c})\chi_\Lambda(dx_\Lambda), \tag{2.85}$$

which is a probability measure on Ω^t. Then

$$\pi^{\mathrm{per}}_\Lambda(d(\omega_\Lambda \times \omega_{\Lambda^c})) = \nu^{\mathrm{per}}_\Lambda(d\omega_\Lambda)\prod_{\square'\square\Lambda^c}\delta_{0_{\square'}}(dx_{\square'}), \tag{2.86}$$

where $0_{\square'}$ is the zero element of the Banach space

of the pressure on the external field h, c.f. (2.3), we indicate this dependence explicitely. For $\Lambda \Subset \mathsf{L}$, we set, see (2.49),

$$p_\Lambda(h,\xi) = \frac{1}{|\Lambda|}\log N_\Lambda(h,\xi), \quad \xi \in \Omega^t. \tag{2.88}$$

To simplify notations we write $p_\Lambda(h) = p_\Lambda(h,0)$. Thereby, for $\mu \in G^t$, we set

$$p^\mu_\Lambda(h) = \int_\Omega p_\Lambda(h,\xi)\mu(d\xi). \tag{2.89}$$

Furthermore, we set

$$p^{\mathrm{per}}_\Lambda(h) = \frac{1}{|\Lambda|}\log N^{\mathrm{per}}_\Lambda(h). \tag{2.90}$$

If, for a cofinal sequence L, the limit

$$p^\mu(h) \stackrel{\mathrm{def}}{=} \lim_{\mathsf{L}} p^\mu_\Lambda(h) \tag{2.91}$$

exists, we call it pressure in the state μ)

$$\stackrel{\mathrm{d}}{=} \qquad \Lambda)(h$$

The same representation can also be written for $\mathbf{N}_\Lambda^{\rm per}(\mathbf{h})$. One can show that the pressures $\mathbf{p}_\Lambda(\mathbf{h})$ and $\mathbf{p}_\Lambda^{\rm per}(\mathbf{h})$, as functions of $\mathbf{h}$, are analytic in a subset of C, which contains R. Thus, one can compute the derivatives and obtain

$$\frac{\partial}{\partial \mathbf{h}}\mathbf{p}_\Lambda(\mathbf{h}) = \beta \mathbf{M}_\Lambda(\mathbf{h}), \qquad \frac{\partial}{\partial \mathbf{h}}\mathbf{p}_\Lambda^{\rm per}(\mathbf{h}) = \beta \mathbf{M}_\Lambda^{\rm per}(\mathbf{h}), \tag{2.96}$$

where

$$\mathbf{M}_\Lambda(\mathbf{h}) \stackrel{\rm def}{=} \frac{1}{|\Lambda|}\sum_{\square\square\Lambda} \square_\Lambda[\mathbf{q}_\square^{(1)}], \quad \mathbf{M}_\Lambda^{\rm per}(\mathbf{h}) \stackrel{\rm def}{=} \square_\Lambda^{\rm per}[\mathbf{q}_\square^{(1)}] \tag{2.97}$$

are local *polarizations*, corresponding to the zero and periodic boundary conditions respectively. Furthermore,

$$\frac{\partial^2}{\partial \mathbf{h}^2}\mathbf{p}_\Lambda(\mathbf{h}) \tag{2.98}$$
$$= \frac{1}{2|\Lambda|}\int_{\Omega_\Lambda}\int_{\Omega_\Lambda}\sum_{\square\square\Lambda}\int_0^\beta \square\left(\omega_\square^{(1)}(\tau) - \tilde\omega_\square^{(1)}(\tau)\right)^2 d\tau \; \nu_\Lambda(d\omega_\Lambda)\nu_\Lambda(d\tilde\omega_\Lambda) \geq 0.$$

The same can be said about the second derivative of $\mathbf{p}_\Lambda^{\rm per}(\mathbf{h})$. Therefore, both $\mathbf{p}_\Lambda(\mathbf{h})$ and $\mathbf{p}_\Lambda^{\rm per}(\mathbf{h})$ are convex functions. For the reader convenience, we present here the corresponding properties of convex functions following [69], pages 34 - 37.

For a function $\boldsymbol{\phi} : \mathsf{R} \to \mathsf{R}$, by $\boldsymbol{\phi}'_\pm(\mathbf{t})$ we denote its one-side derivatives at a given $\mathbf{t} \in \mathsf{R}$. By *at most countable set* we mean the set which is void, finite, or countable.

Proposition 2.24 *For a convex function $\boldsymbol{\phi} : \mathsf{R} \to \mathsf{R}$, it follows that:*

(a) the dehe dehe dehe d.(697.2197(t)-5.v9.239849.076(d)5.2197(e3.592197(t)-5.v9.239849.96264Tf9115(

3.1 Phase transitions and order parameters

We begin by introducing the main notion of this section.

Definition 3.1

Proof: By (3.9), $\hat{B}(p)\cos(p, x - x')$ is an absolutely integrable function in the sense of improper Riemann integral. The right-hand side of (3.11) is its integral sum; thereby, the convergence stated is obtained in a standard way. □

From claim (i) of (3.9) by the Riemann-Lebesgue lemma, see page 116 in [55], one obtains

$$\lim_{|x - x'| \to +\infty} B_{xx'} = 0. \tag{3.12}$$

Lemma 3.3 *For every box* Λ *and any* $x, x' \in \Lambda$, *it follows that*

$$D^{\Lambda}_{xx'} \geq \tfrac{1}{2}\left[D^{\Lambda}_{xx} - B^{\Lambda}_{xx} \right] + B^{\Lambda}_{xx'}. \tag{3.13}$$

Proof: By (3.7), (3.11), and claim (ii) of (3.9), one has

$$D^{\Lambda}_{xx} - D^{\Lambda}_{xx'} = \frac{2}{|\Lambda|} \sum_{p \in \Lambda_0 \setminus \{0\}} \hat{D}^{\Lambda}_{p} \sin^2

Let us consider now another possibilities to define phase transitions in translation invariant versions of our model. For a box Λ, see (2.63), we introduce

$$\begin{aligned} \mathbf{P}_\Lambda &= \frac{1}{(\beta|\Lambda|)^2} \sum_{\square,\square' \square \Lambda} \mathbf{D}^{\Lambda}_{\square\square'} \\ &= \int_{\Omega_\Lambda} \left[\frac{1}{\beta|\Lambda|} \sum_{\square\square\Lambda} \int_0^\beta \omega_\square(\tau) d\tau \right]^2 \nu^{\mathrm{per}}_\Lambda(d\omega_\Lambda), \end{aligned} \tag{3.19}$$

and set

$$\mathbf{P} \stackrel{\mathrm{def}}{=} \limsup_{L \to +\infty} \mathbf{P}_{\Lambda_L}. \tag{3.20}$$

Definition 3.5 *The above* $\mathbf{P}$ *is called the order parameter. If* $\mathbf{P} > 0$ *for*

Proposition 3.9 (Gri ths) *Let the sequence of measures* $\{\mu_n\}_{n\in\mathbb{N}}$ *be as above. If* $f'_+(0) = f'_-(0) = \varphi$ *(i.e.,* f *is di erentiable at* $y = 0$*), then*

$$\lim_{n\to+\infty} \int g(u/M_n)\mu_n(du) = g(\varphi), \tag{3.22}$$

for any continuous $g : \mathbb{R} \to \mathbb{R}$*, such that* $|g(u)| \le \lambda e^{\varkappa|u|}$ *with certain* $\lambda, \kappa > 0$

Proposition 3.10 *If there exists* α $\square$

3.2 Infrared bound

Taking this into account we obtain

$$\bar{Q}_{\square\square_1,\square_1'\square\square_2,\square_2'\square}(\mathbf{k}) = \sum_{\mathbf{p}\square\Lambda_\square} \square\hat{\omega}^{(\mathbf{j})}(\mathbf{p},\mathbf{k})\hat{\omega}^{(\mathbf{j})}(-\mathbf{p},\mathbf{k})\square_{\nu^{\mathrm{per}}_{\beta,\Lambda}} \times \left[e^{\imath(\mathbf{p},\square_1)} - e^{\imath(\mathbf{p},\square_1')}\right] / |\Lambda|^{1/2} \times \left[e^{-\imath(\mathbf{p},\square_2)} - e^{\imath(-\mathbf{p},\square_2')}\right] / |\Lambda|^{1/2}. \tag{3.48}$$

Since the summand corresponding to $\mathbf{p} = 0$ equals zero, the sum can be restricted to $\Lambda_\square \setminus \{0\}$. This representation however cannot serve as a spectral decomposition similar to (3.45) because the eigenfunctions here are not normalized. Indeed,

$$\sum_{\square\square,\square'\square\square\mathbf{E}} \left[e^{\imath(\mathbf{p},\square)} - e^{\imath(\mathbf{p},\square')}\right] / |\Lambda|^{1/2} \times \left[e^{-\imath(\mathbf{p},\square)} - e^{-\imath(\mathbf{p},\square')}\right] / |\Lambda|^{1/2} = 2\mathbf{E}(\mathbf{p})$$

where

$$\mathbf{E}(\mathbf{p}) \stackrel{\mathrm{def}}{=} \sum_{\mathbf{j}=1}^{\mathbf{d}} [1 - \cos \mathbf{p}_\mathbf{j}]. \tag{3.49}$$

Then we set

$$\sigma_{\square\square'}(\mathbf{p}) = \left[e^{\imath(\mathbf{p},\square)} - e^{\imath(\mathbf{p},\square')}\right] / \sqrt{2|\Lambda|\mathbf{E}(\mathbf{p})}, \quad \mathbf{p} \square \Lambda_\square \setminus \{0\}, \tag{3.50}$$

and

$$\bar{Q}(\mathbf{p},\mathbf{k}) = 2\mathbf{E}(\mathbf{p})\square\hat{\omega}^{(\mathbf{j})}(\mathbf{p},\mathbf{k})\hat{\omega}^{(\mathbf{j})}(-\mathbf{p},\mathbf{k})\square_{\nu^{\mathrm{per}}_{\Lambda}}, \quad \mathbf{p} \square \Lambda_\square \setminus \{0\}. \tag{3.51}$$

Thereby,

$$Q_{\square\square_1,\square_1'\square\square_2,\square_2'\square}(\tau,\tau') = \sum_{\square} = \sum_{\mathbf{p}\square\Lambda_\square\setminus\{0\}} \sum_{\mathbf{k}\square\mathbf{K}} \bar{Q}(\mathbf{p},\mathbf{k})\sigma_{\square_1\square_1'}(\mathbf{p})\sigma_{\square_2\square_2'}(-\mathbf{p})e_\mathbf{k}(\tau)e_\mathbf{k}(\tau'), \tag{3.52}$$

which is the spectral decomposition of the operator (3.39). Now we show that the eigenvalues (3.51) have a specific upper bound[4].

Lemma 3.13 *For every* $\mathbf{p} \square \Lambda_\square \setminus \{0\}$ *and* $\mathbf{k} \square \mathbf{K}$*, the eigenvalues (3.51) obey the estimate*

$$\bar{Q}(\mathbf{p},\mathbf{k}) \le 1/\mathbf{J}, \tag{3.53}$$

where $\mathbf{J}$ *is the same as in (3.32). From this estimate one gets*

$$\square\hat{\omega}^{(\mathbf{j})}(\mathbf{p},\mathbf{k})\hat{\omega}^{(\mathbf{j})}(-\mathbf{p},\mathbf{k})\square_{\nu^{\mathrm{per}}_{\Lambda}} \le \frac{1}{2\mathbf{J}\mathbf{E}(\mathbf{p})}, \quad \mathbf{p} \square \Lambda_\square \setminus \{0\}. \tag{3.54}$$

Proof: The estimate in question will be obtained from the Gaussian domination (3.36). For $\mathbf{t} \square \mathbf{R}$ and a given $\mathbf{b} \square \mathbf{X}_\mathbf{E}$, we consider the function $\varphi(\mathbf{t}) = \mathbf{Y}_\Lambda(\mathbf{tb})$. By Lemma 3.12, $\varphi''(0) \le 0$. Computing the derivative from (3.35) we get

$$\varphi''(0) = \mathbf{J}(\mathbf{b},\mathbf{Qb})_{\mathbf{X}_\mathbf{E}} - \square\mathbf{b}\square^2_{\mathbf{X}_\mathbf{E}},$$

[4]Their natural lower bound is zero as the operator (3.39) is positive

Then we take in (3.59) $\mathbf{A} = \mathbf{p}_{\square}^{(\mathbf{j})}$, $\mathbf{j} = 1$

3.4 Phase transition in the symmetric scalar models

In the case $\nu = 1$, we can extend the above results to the models without translation invariance and with much more general $J_{\square\square'}$ and $V_{\square}$. However, certain assumptions beyond (2.1) and (2.2) should be made. Suppose also that the interaction between the nearest neighbors is uniformly nonzero, i.e.,

$$\inf_{|\square - \square'|=1} J_{\square\square'} \stackrel{\text{def}}{=} J > 0. \tag{3.76}$$

Next we suppose that all $V_{\square}$ a-is

imposed on the anharmonic potential is (2.2). Obviously, we have to include the external field, that is the anharmonic potential is now $V(u) - hu$. Since we are not going to impose any conditions on the odd part of V, we cannot apply the GKS inequalities, see [6, 54], the comparison methods are based on, see (3.84). In view of this fact we suppose that the interaction is of nearest neighbor type. Thus, for a box Λ, the periodic local Hamiltonian of the model has the form (3.81).

In accordance with Definition 3.7, our goal is to show that the model parameters (except for h) and the inverse temperature β can be chosen in such a way that the set R, defined by (2.100), is non-void. The main idea on how to do this can be explained as follows. First we find a condition, independent of h, under which $D^{\mu}_{\Box\Box^{\Box}}$ does not decay to zero for a certain periodic μ. Next we prove the following

Lemma 3.23 *There exist* $h_{\pm}$, $h_{-} < h_{+}$, *which may depend on the model parameters and* β, *such that the magnetization (2.101) has the property:*

$$M(h) < 0, \quad \text{for} \quad h \in R^{c} \cap (-\infty, h_{-}); \qquad M(h) > 0, \quad \text{for} \quad h \in R^{c} \cap (h_{+} + \infty).$$

Thereby, if R were void, one would find $h_{\Box} \in (h_{-}, h_{+})$ such that $M(h_{\Box}) = 0$. At such $h_{\Box}$, the aforementioned property of D^{μ} would yield the non-ergodicity of μ and hence the first order phase transition, see Theorem 3.22.

In view of Corollary 3.4, $D^{\mu}_{\Box\Box^{\Box}}$ does not decay to zero if (3.16) holds with big enough ϑ. By Proposition 3.18, the lower bound (3.16) can be obtained from the estimate (3.61). The only problem with the latter estimate is that it holds for $h = 0$.

Lemma 3.24 *For every* $\beta > 0$ *and* θ, *there exist positive* $m_{\Box}$ *and* $J_{\Box}$, *which may depend on* $\beta > 0$ *and* θ *but are independent of* h, *such that, for any box* Λ *and any* $h \in R$,

$$\Big[\omega_{\Box}(0)\Big]^{2}_{\nu^{\mathrm{per}}_{\Lambda}} \geq \theta, \quad \text{if} \quad J > J_{\Box} \ \text{ and } \ m > m_{\Box}. \tag{3.85}$$

Proof: For $h \in R$, we set

$$\lambda^{h}(d\omega) = \frac{1}{N^{h}_{\beta}} \exp\Big\{ h \int_{0}^{\beta} \omega(\tau) d\tau \Big\} \lambda(d\omega), \tag{3.86}$$

$$N^{h}_{\beta} = \int_{C_{\beta}} \exp\Big\{ h \int_{0}^{\beta} \omega(\tau) d\tau \Big\} \lambda(d\omega),$$

where λ is as in (2.102). Then for $\pm h > 0$, we get the estimate (3.64) in the following form

$$\beta J d \Big[\omega_{\Box}(0)\Big]^{2}_{\nu^{\mathrm{per}}_{\Lambda}} \geq \beta J d\varepsilon^{2} + \log \lambda^{h}\Big[B^{\pm}(\varepsilon, c)\Big], \tag{3.87}$$

where $B^{\pm}(\varepsilon, c)$ is as in (2.108), (2.109). Let us show now that, for $\pm h \geq 0$,

$$\lambda^{h}\Big[B^{\pm}(\varepsilon, c)\Big] \geq \lambda\Big[B^{\pm}(\varepsilon, c)\Big]. \tag{3.88}$$

For $h \geq 0$, let $I(\omega)$ be the indicator function of the set $C^{+}_{\beta}(n; c)$, see (2.106). For $\delta > 0$ and $t \in R$, we set

$$\iota_{\delta}(t) = \begin{cases} 0 & t \leq c, \\ (t - c)/\delta & t \in (c, c + \delta], \\ 1 & c \geq c + \delta. \end{cases}$$

Thereby,

$$I_\delta(\omega) \stackrel{\mathrm{def}}{=} \prod_{k=0}^{n} I_\delta\left[\omega(k\beta/n)\right].$$

By Lebesgue's dominated convergence theorem

$$N_\beta^h \lambda^h\left(C_\beta^+(n;c)\right) = \int_{C_\beta} I(\omega) \exp\left\{h \int_0^\beta \omega(\tau)d\tau\right\} \lambda(d\omega) \qquad (3.89)$$

$$= \lim_{\delta\downarrow 0} \int_{C_\beta} I_\delta(\omega) \exp\left\{h \int_0^\beta \omega(\tau)d\tau\right\} \lambda(d\omega).$$

As the function I_δ is continuous and increasing, by the FKG inequality, see Theorem 6.1 in [6], it follows that

$$\int_{C_\beta} I_\delta(x) \exp\left\{h \int_0^\beta \omega(\tau)d\tau\right\} \lambda(d\omega) \geq N_\beta^h \int_{C_\beta} I_\delta(\omega)\lambda(d\omega).$$

Passing here to the limit we obtain from (3.89)

$$\lambda^h\left(C_\beta^+(n;c)\right) \geq \lambda\left(C_\beta^+(n;c)\right),$$

which obviously yields (3.88). For $h \leq 0$, one just changes the signs of h and ω. Thereby, we can rewrite (3.87) as follows, c.f., (3.64),

$$\int [\omega(0)]^2 \, \nu_\Lambda^{\mathrm{per}} \geq \varepsilon^2 + [\log\gamma(m)]/\beta J d.$$

Then one applies the arguments from the very end of the proof of Lemma 3.16. □

Proof of Lemma 3.23: Suppose that $h >$

Proof: Let $m_\square$ be as in (2.110) and $J_\square$, θ be as in Lemma 3.24. Fix any $\beta > 0$ and $m > m_\square$. Then, for $J > J_\square$

in [24]. For translation invariant models with bounded interaction, non-di erentiability of the pressure corresponds to the non-uniqueness of the Gibbs states, see [36, 69]. We failed to prove this for our model.

In the language of limit theorems of probability theory, the appearance of the long range order corresponds to the fact that a new law of large numbers comes to power, see Theorem 3.9 and the discussion preceding Definition 3.11. The critical point of the model corresponds to the case where the law of large numbers still holds in its original form (in the translation invariant case this means absence of the first order phase transitions), but the central limit theorem holds true with an abnormal normal

The latter condition can be satisfied by picking big enough β. Therefore, the classical anharmonic crystals always have phase transitions – no matter how small is the interaction intensity. For finite m, the left-hand side of (4.4) is bounded by $8m\vartheta_0^2 J$, and the bound is achieved in the limit $\beta \to +\infty$. If for given values of the interaction parameter J, the mass m, and the parameter ϑ_0 which characterizes the anharmonic potential, this bound does not exceed $J(d)$, the condition (4.4) will never be satisfied. Although this condition is only sufficient, one might expect that the phase transition can be eliminated at all β if the compound parameter $8m\vartheta_0^2 J$ is small enough. Such an effect, if really exists, could be called *quantum stabilization* since it is principally impossible in the classical analog of the model.

4.2 Quantum rigidity

In the harmonic case, big values of the rigidity a ensure the stability. In this subsection, we introduce and stugy *quantum rigidity*, which plays a similar role in the anharmonic case

Above the sufficient condition (4.4) for a phase transition to occur was obtained for a simplified version of the model (1.1), (1.2) – nearest neighbor interactions, polynomial anharmonic potentials of special kind (3.78), ect. Then the results were extended to more general models via correlation inequalities. Likewise here, we start with a simple scalar version of the one-particle Hamiltonian (1.1), which we take in the form

$$H_m = \frac{1}{2m}p^2 + \frac{a}{2}q^2 + V(q$$

Proof: Given $\alpha > 0$, let $U_\alpha : L^2(R) \to L^2(R)$ be the following unitary operator

$$(U_\alpha \psi)(x) = \sqrt{\alpha}\psi(\alpha x). \tag{4.18}$$

where

$$H_{m_0}^{(0)} = \frac{1}{2m_0}p^2 + b^{(r)}q^{2r},$$

and

$$R(\rho) = \rho^{r-2}(b^{(1)} + a/2)q^2 + \rho^{r-3}b^{(2)}q^4 + \cdots + b^{(r-1)}q^{2(r-1)}.$$

Repeating the above perturbation arguments one concludes that the self-adjoint family $\{\hat{}$

where $\mathbf{Z_m}$

4.4 Decay of correlations in the scalar case

In this subsection, we consider the model (1.1), (1.2) which is (a) translation invariant; (b) scalar; (c) the anharmonic potential is $V(q) = v(q^2)$ with v being convex on R_+.

Let Λ be the box (2.63) and $\Lambda_\square$ be its conjugate (3.2). For this Λ, let

$$K^{\Lambda}_{\square\square'}(\tau,\tau') \stackrel{\text{def}}{=} \langle \omega_\square(\tau)\omega_{\square'}(\tau')\rangle^{\square}_{\nu^{\text{per}}_\Lambda} \tag{4.34}$$

be the periodic correlation function. Recall that the periodic interaction potential $J^{\Lambda}_{\square\square'}$ was defined by (2.78). For the one-particle Hamiltonian (1.2), let $\hat{u}(k)$ be as in (4.28).

Theorem 4.4 *Let the model be as just describes. If*

$$\hat{u}(0)\hat{J}_0 < 1, \tag{4.35}$$

then

$$K^{\Lambda}_{\square\square'}(\tau,\tau') \le \frac{1}{\beta|\Lambda|}\sum_{p\in\Lambda_\square}\sum_{k\in K}\frac{\exp[\imath(p,\square-\square')+\imath k(\tau-\tau')]}{[\hat{u}(k)]^{-1}-\hat{J}^{\Lambda}_0+Y^{\Lambda}(p)}, \tag{4.36}$$

where

$$\hat{J}^{\Lambda}_0 = \sum_{\square'\in\Lambda} J^{\Lambda}_{\square\square'}, \qquad Y^{\Lambda}(p) = \hat{J}^{\Lambda}_0 - \sum_{\square'\in\Lambda} J^{\Lambda}_{\square\square'}\exp[\imath(p,\square-\square')]. \tag{4.37}$$

Proof: Along with the periodic local Gibbs measure (2.82) we introduce

$$\begin{aligned}&\nu^{\text{per}}_\Lambda(d\omega_\Lambda|t) \\ &= \frac{1}{N^{\text{per}}_\Lambda(t)}\exp\Big[\frac{t}{2}\sum_{\square,\square'\in\Lambda} J^{\Lambda}_{\square\square'}(\omega_\square,\omega_{\square'})_{L^2_\beta} - \int_0^\beta\sum_{\square\in\Lambda} V(\omega_\square(\tau))d\tau\Big]\chi_\Lambda(d\omega_\Lambda),\end{aligned} \tag{4.38}$$

where $t \in [0,1]$ and $N^{\text{per}}_\Lambda(t)$ is the corresponding normalization factor. Thereby, we set

$$X_{\square\square'}(\tau,\tau'|t) = \langle\omega_\square(\tau)\omega_{\square'}(\tau')\rangle_{\nu^{\text{per}}_\Lambda(\cdot|t)}, \quad \square,\square' \in \Lambda. \tag{4.39}$$

By direct calculation

$$\begin{aligned}\frac{\partial}{\partial t}X_{\square\square'}(\tau,\tau'|t) &= \frac{1}{2}\sum_{\square_1,\square_2\in\Lambda} J^{\Lambda}_{\square_1\square_2}\int_0^\beta R_{\square\square'\square_1\square_2}(\tau,\tau',\tau'',\tau''|t)d\tau'' \\ &+ \sum_{\square_1,\square_2\in\Lambda} J^{\Lambda}_{\square_1\square_2}\int_0^\beta X_{\square\square_1}(\tau,\tau''|t)X_{\square_2\square'}(\tau'',\tau'|t)d\tau'',\end{aligned} \tag{4.40}$$

where

$$\begin{aligned}R_{\square_1\square_2\square_3\square_4}(\tau_1,\tau_2,\tau_3,\tau_4|t) &= \langle\omega_{\square_1}(\tau_1)\omega_{\square_2}(\tau_2)\omega_{\square_3}(\tau_3)\omega_{\square_4}(\tau_4)\rangle_{\nu^{\text{per}}_\Lambda(\cdot|t)} \\ &- \langle\omega_{\square_1}(\tau_1)\omega_{\square_2}(\tau_2)\rangle_{\nu^{\text{per}}_\Lambda(\cdot|t)}\cdot\langle\omega_{\square_3}(\tau_3)\omega_{\square_4}(\tau_4)\rangle_{\nu^{\text{per}}_\Lambda(\cdot|t)} \\ &- \langle\omega_{\square_1}(\tau_1)\omega_{\square_3}(\tau_3)\rangle_{\nu^{\text{per}}_\Lambda(\cdot|t)}\cdot\langle\omega_{\square_2}(\tau_2)\omega_{\square_4}(\tau_4)\rangle_{\nu^{\text{per}}_\Lambda(\cdot|t)} \\ &- \langle\omega_{\square_1}(\tau_1)\omega_{\square_4}(\tau_4)\rangle_{\nu^{\text{per}}_\Lambda(\cdot|t)}\cdot\langle\omega_{\square_2}(\tau_2)\omega_{\square_3}(\tau_3)\rangle_{\nu^{\text{per}}_\Lambda(\cdot|t)}.\end{aligned}$$

for all $\mathbf{p} \in \Lambda_\sigma$ and $\mathbf{k} \in \mathbf{K}$. Thus, the problem (4.48) can be solved explicitly, which via the transformation (4.47) yields (4.46).

Given $\theta \in (0,1)$, we set

$$Y^{(\theta)}_{\sigma\sigma'}(\tau,\tau'|t) = Y_{\sigma\sigma'}(\tau,\tau'|t+\theta), \quad t \in [0,1-\theta]. \tag{4.50}$$

Obviously, the latter function obeys the equation (4.44) on $t \in [0,1-\theta]$ with the initial condition

$$Y^{(\theta)}_{\sigma\sigma'}(\tau,\tau'|0) = Y_{\sigma\sigma'}(\tau,\tau'|\theta) > Y_{\sigma\sigma'}(\tau,\tau'|0) = X_{\sigma\sigma'}(\tau,\tau'|0). \tag{4.51}$$

The latter inequality is due to the positivity of both sides of (4.44). Therefore,

$$Y^{(\theta)}_{\sigma\sigma'}(\tau,\tau'|t) > 0, \tag{4.52}$$

for all $\sigma,\sigma' \in \Lambda$, $\tau,\tau' \in [0,\beta]$, and $t \in [0,1-\theta]$.

Let us show now that under the condition (4.35), for all $\theta \in (0,1)$ and $\varepsilon \in (0,\varepsilon_0)$,

$$X_{\sigma\sigma'}(\tau,\tau'|t) < Y^{(\theta)}_{\sigma\sigma'}(\tau,\tau'|t), \tag{4.53}$$

also for all $\sigma,\sigma' \in \Lambda$, $\tau,\tau' \in [0,\beta]$, and $t \in [0,1-\theta]$. To this end we introduce

$$Z^{\pm}_{\sigma\sigma'}(\tau,\tau'|t) \stackrel{\text{def}}{=} Y^{(\theta)}_{\sigma\sigma'}(\tau,\tau'|t) \pm X_{\sigma\sigma'}(\tau,\tau'|t), \quad t \in [0,1-\theta]. \tag{4.54}$$

Then one has from (4.40), (4.44)

$$\begin{aligned}
&\frac{\partial}{\partial t} Z^{-}_{\sigma\sigma'}(\tau,\tau'|t) \qquad\qquad (4.55)\\
&= \frac{1}{2} \sum_{\sigma_1,\sigma_2 \in \Lambda} J^{\Lambda}_{\sigma_1\sigma_2} \int_0^\beta \Big[Z^{+}_{\sigma\sigma_1}(\tau,\tau''|t) Z^{-}_{\sigma'\sigma_2}(\tau',\tau''|t)\\
&+ Z^{-}_{\sigma\sigma_1}(\tau,\tau''|t) Z^{+}_{\sigma'\sigma_2}(\tau',\tau''|t) \Big] d\tau''\\
&+ \frac{\varepsilon}{|\Lambda|} \sum_{\sigma_1,\sigma_2 \in \Lambda} \int_0^\beta Y^{(\theta)}_{\sigma\sigma_1}(\tau,\tau''|t) Y^{(\theta)}_{\sigma'\sigma_2}(\tau',\tau''|t) d\tau'' - S_{\sigma\sigma'}(\tau,\tau'|t),
\end{aligned}$$

where $S_{\sigma\sigma'}(\tau,\tau'|t)$ stands for the first term on the right-hand side of (4.40). By (4.54) and (4.51)

$$Z^{-}_{\sigma\sigma'}(\tau,\tau'|0) = Y_{\sigma\sigma'}(\tau,\tau'|\theta) - X_{\sigma\sigma'}(\tau,\tau'|0) > 0, \tag{4.56}$$

which holds for all $\sigma,\sigma' \in \Lambda$, $\tau,\tau' \in [0,\beta]$. For every $\sigma,\sigma' \in \Lambda$, both $Y_{\sigma\sigma'}(\tau,\tau'|t)$, $X_{\sigma\sigma'}(\tau,\tau'|t)$ and, hence, $Z^{\pm}_{\sigma\sigma'}(\tau,\tau'|t)$ are continuous functions of their arguments. Set

$$\zeta(t) = \inf \Big\{ Z^{-}_{\sigma\sigma'}(\tau,\tau'|t) \;\Big|\; \sigma,\sigma' \in \Lambda, \;\; \tau,\tau' \in [0,\beta] \Big\}. \tag{4.57}$$

By (4.56), it follows that $\zeta(0) > 0$. Suppose now that $\zeta(t_0) = 0$ at some $t_0 \in [0,1-\theta]$ and $\zeta(t) > 0$ for all $t \in [0,t_0)$. Then by the continuity of $Z^{-}_{\sigma\sigma'}$, there exist $\sigma,\sigma' \in \Lambda$ and $\tau,\tau' \in [0,\beta]$ such that

$$Z^{-}_{\sigma\sigma'}(\tau,\tau'|t_0) = 0 \quad \text{and} \quad Z^{-}_{\sigma\sigma'}(\tau,\tau'|t) > 0 \quad \text{for all } t < t_0.$$

For these $\sigma,\sigma' \in \Lambda$ and $\tau,\tau' \in [0,\beta]$, the derivative $(\partial/\partial t) Z^{-}_{\sigma\sigma'}(\tau,\tau'|t)$ at $t = t_0$ is positive since on the right-hand side of (4.55) the third term is positive and

the remaining terms are non-negative. But a differentiable function, which is positive at $t \in [0, t_0)$ and zero at $t = t_0$, cannot increase at $t = t_0$. Thus, $\zeta(t) > 0$ for all $t \in [0, 1 - \theta]$, which yields (4.53). By the latter estimate, we have

$$X_{\sigma\sigma'}(\tau, \tau' | 1 - \theta) < Y_{\sigma\sigma'}(\tau, \tau' | 1) = \frac{1}{\beta |\Lambda|} \sum_{p \in \Lambda_*} \sum_{k \in K} \frac{\exp[i(p, x - x') + ik(\tau - \tau')]}{[\hat{u}(k)]^{-1} - t[\hat{J}_0^{\Lambda} + \varepsilon \delta_{p,0}] + t Y^{\Lambda}(p)}.$$

All the function above depend on θ and ε continuously. Hence, passing here to the limit $\theta = \varepsilon \downarrow 0$ and taking into account (4.43) we obtain (4.36). $\square$

By means of Proposition 2.21, the result just proven can be extended to all periodic elements of G^t. For $\mu \in G^t$, we set

$$K^{\mu}_{\sigma\sigma'}(\tau, \tau') = \omega_{\sigma}(\tau) \omega_{\sigma'}(\tau')_{\mu}. \tag{4.58}$$

Theorem 4.5 *Let the stability condition (4.16) be satisfied. Then for every periodic* $\mu \in G^t$

4.5 Decay of correlations in the vector case

In the vector case, the eigenvalues of the Hamiltonian (4.5) are no longer simple;

In the scalar case, the most general result is the following statement, see Theorem 3.13 in [54].

Theorem 4.10

If Λ is a box, the parameter (3.28) can be written

$$P_{\Lambda}^{(\alpha)} = \frac{1}{\beta^2 |\Lambda|^{\alpha}} \sum_{j=1}^{\nu} \int_0^{\beta} \int_0^{\beta} \Gamma^{\beta,\Lambda}_{Q_{\Lambda}^{(j)},Q_{\Lambda}^{(j)}}(\tau,\tau')\,d\tau\,d\tau'. \tag{4.67}$$

Thus, if the fluctuations are normal, phase transitions of the second order (and all the more of the first order) do not occur.

Like in the proof of Theorem 4.9, the model is compared with the scalar ferromagnetic model with the same mass and the anharmonic potential $v(q^2)$. Then the gap parameter Δ_m is the one calculated for the latter model.

Theorem 4.12

$m\Delta_m^2$ was called quantum rigidity and the e ect was called quantum stabilization. If the tunneling between the wells gets more intensive (closer minima), or if the mass diminishes, $m\Delta_m^2$ gets bigger and the particle 'forgets' about the details of the potential energy in the vicinity of the origin (including instability) and oscillates as if its equilibrium at zero is stable, like in the harmonic case.

- *Subsection 4.3:* Theorems 4.2 and 4.3 are new. Preliminary results of this kind were obtained in [3, 50].
- *Subsection 4.4:* Theorems 4.4, 4.5, 4.7 were proven in [45].
- *Subsection 4.5:* Various scalar domination estimates were obtained in [47, 48, 49].
- *Subsection 4.6:* Theorem 4.10 was proven in [54]. The proof of Theorem 4.12 was done in [49]. The suppression of abnormal fluctuations in the hierarchical version of the model (1.1), (1.2) was proven in [2].

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