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Fluctuations in an asymmetric anharmonic crystal

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Abstract. In this paper we continue the investigation of the structural phase transition in a quantum anharmonic crystal. We calculate the influence of breaking the symmetry of the interaction potential on the behaviour of fluctuations and their critical exponents. More precisely, it is shown that when the low-momentum asymptotics of the phonon spectrum (i.e. the Fourier transform of the interaction matrix) have a quartic asymptotic in one direction, the critical exponents for the momentum and position fluctuations increase on the critical line. The quantum nature of the fluctuations in $T = 0$ is, however, preserved.

1. Introduction

Fluctuations are inherently connected with critical phenomena. The standard opinion on the theory of critical phenomena is that fluctuations in a critical point dominate over quantum effects and that critical fluctuations behave in a classical manner ('washing out' of quantum effects by long-range correlations). In most situations, this is in fact the case; but sometimes (especially at low temperatures) the quantum effects can manifest themselves in a macroscopic manner and should be taken into account.

A natural problem where such a competition of effects takes place, is the problem of the displacive phase transitions.

This problem attracted considerable attention from both experimentalists and theoreticians. Experimental evidence exists of quantum effects observed in critical fluctuations in crystals such as $SrTiO_3$ [1]. Theoretical *anharmonic crystal models* intending to deal with such situations were introduced in [4, 8, 2]; the model considered here is borrowed from [2]. In this model, we have a crystal lattice of atoms in a potential which is a superposition of harmonic and double-well-type ones; this model and its solution are presented in section 2.

The theory of fluctuations in quantum systems has been elaborated in a series of papers [5–7]. Within this framework, the notion of the fluctuation as an observable, and a fluctuation operator (corresponding to some physical observable) were introduced. Moreover, the method of how to compute the commutator of two fluctuation operators, and the notions of normality (subnormality, supernormality) were introduced there. Excerpts of this theory, necessary for our paper are presented in section 3.

In this paper, we consider some version of the anharmonic crystal model. Other versions were considered in [2, 3]. To describe how they are related to ours, let us briefly present some results of [2].

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The parameters of the model are $\lambda \equiv \hbar/\sqrt{m}$ (where m denotes the mass of the atoms) and the temperature T. In [2] the full analysis of the phase diagram on a plane (λ, T) was performed. This plane is divided into four regions: a one-phase one (T and λ large), two-phase (T and λ small) and the critical line dividing these regions, with a distinguished point at $T = 0$. In [2], the behaviour of the fluctuation operators (i.e. their commutation properties and the critical exponents δ characterizing deviation from normality) was calculated. The operators in question corresponded to the observables: momentum, displacement and the square of displacement. The results turned out to be dimension dependent, in some cases they also depended on boundary conditions. The quantum effects manifested themselves in the fourth region (i.e. at $T = 0$ on the critical line).

One can expect that the behaviour of a model also depends on the range of interactions. In [3] long-range interactions were considered. The influence of the range on the behaviour of the model on the critical line was examined.

In this paper, a different direction of investigation has been undertaken. We assumed short-range interactions (as in [2]), but an additional assumption was that the low-momentum asymptotic of the phonon spectrum (i.e. of Fourier transform of interaction matrix) was different from the standard one. Normally, this asymptotic is quadratic; however, for some particular values of interaction constants it can happen that the quadratic term vanishes and the asymptotics are quartic or higher order. In this paper, we assume a quartic asymptotic in one direction, and the standard quadratic in other directions. This assumption was motivated by the results of [12], where a non-standard critical behaviour of the spherical model was obtained, when the interaction constants fulfil some special relation. This relation was equivalent to non-standard (non-quadratic) asymptotics of the eigenvalues of interaction matrix. Briefly speaking, it turns out that *the non-standard asymptotic has led to the values of critical exponents δ different than in* [2].

This paper is organized as follows. In section 2 we define the model and recall its thermodynamic properties and phase diagram. We also define there the properties of interactions. The definition and properties of the fluctuation operators are collected in section 3. In section 4 we formulate and prove our main results, concerning properties of the critical fluctuation operators for momenta, displacement and its square on the critical line. We discuss our results in section 5. In the appendix we collect some technical results (asymptotic behaviour of integrals) necessary for the analysis of the gap equation in section 4.

2. Definition of the model and its properties

We consider a model invented to study displacive structural phase transitions with general anharmonicity [4, 8], and exactly solved in [2]. Let us consider a d-dimensional square lattice $\mathbb{Z}^d$. With each lattice point $l \in \mathbb{Z}^d$ we associate a quantum particle with mass m, position Q_l and momentum P_l. The local Hamiltonian H_Λ for any finite subset $\Lambda \in \mathbb{Z}^d$ with $V = |\Lambda|$ is given by the operator

$$H_\Lambda = \sum_{l\in\Lambda} \frac{P_l^2}{2m} + \frac{1}{4}\sum_{l,l'\in\Lambda} \phi_{l-l'}(Q_l - Q_{l'})^2 + \frac{a}{2}\sum_{l\in\Lambda} Q_l^2 + VW\left(\frac{1}{V}\sum_{l\in\Lambda} Q_l^2\right) - h\sum_{l\in\Lambda} Q_l \qquad (1)$$

acting on the Hilbert space $\mathcal{H}_\Lambda = \bigotimes_\Lambda L^2(\mathbb{R}^1)$.

The first and second terms describe (the quantum version of) the Debye approximation. The third term describes the stabilization of the lattice and creates a gap in the phonon spectrum. The fourth one was introduced to describe the displacive phase transition: we assume that $W(x)$ is a function such that the superposition $W(x) + (a/2)x^2$ has a non-degenerate minimum outside $x = 0$. Typical examples of $W(x)$ functions are:

- $W(x) = (b/2)\exp(-\eta|x|)$ with b, η sufficiently large to destabilize the a term;
- the polynomial choice: $W(x) = b(x^4 - \eta x^2)$ with again b, η sufficiently large.

The particular choice is not important for us if the function $W(x)$ fulfils some conditions [4].

Remark. Consider the model with the Hamiltonian H'_Λ of the form (1), but with third and fourth terms replaced by $\sum_{l\in\Lambda}((a/2)Q_l^2 + W(Q_l^2))$. Such a choice gives us a *local* model, which is more realistic, but also much more difficult to deal with. The difference between models described by Hamiltonians H and with H' is similar to the difference between the Ising model and the spherical one. The substitution of Q_l^2 by the arithmetic mean over Λ is an *ansatz* corresponding to the concept of the *self-consistent-phonons* (see [10, 4]).

The model (1) is soluble in the sense that for all temperatures $T \geqslant 0$, the free-energy density and the thermal averages can be calculated explicitly (see [2]). Take the hypercubic subset $\Lambda \subset \mathbb{Z}^d$ with periodic boundary conditions:

$$\Lambda = \left\{ l \in \mathbb{Z}^d \,\middle|\, -\frac{N_\alpha}{2} < l_\alpha \leqslant \frac{N_\alpha}{2}; \alpha = 1, \ldots, d \right\} \tag{2}$$

then $V = \prod_{\alpha=1}^d N_\alpha$ and the dual lattice Λ^* is given by

$$\Lambda^* = \left\{ q \,\middle|\, q_\alpha = \frac{2\pi}{N_\alpha} n^\alpha; n^\alpha = 0, \pm 1, \ldots, \pm\left(\frac{N_\alpha}{2} - 1\right), \frac{N_\alpha}{2}; \alpha = 1, \ldots, d \right\}. \tag{3}$$

The free-energy density for this model is given by

$$f(T, h = 0) = \lim_\Lambda \left\{ \frac{1}{\beta V} \sum_{q\in\Lambda^*} \ln[2\,\mathrm{sh}\,\beta\lambda\Omega_q(c_\Lambda)] + W(c_\Lambda) - c_\Lambda W'(c_\Lambda) \right\} \tag{4}$$

where c_Λ is a solution for c of the self-consistency equation

$$c = \left\langle \frac{1}{V} \sum_{l\in\Lambda} Q_l^2 \right\rangle_{H_\Lambda(c, h=0)} = \frac{1}{V} \sum_{q\in\Lambda^*} \frac{\lambda}{2\Omega_q(c)} \coth \frac{\beta\lambda}{2} \Omega_q(c). \tag{5}$$

Here $\beta = 1/kT$ and

$$\lambda = \frac{\hbar}{\sqrt{m}} \tag{6}$$

$$\Omega_q^2(c) = \omega_q^2 + \Delta(c) \tag{7}$$

$$\Delta(c) = a + 2W'(c) \tag{8}$$

$$\omega_q^2 = \tilde{\phi}(0) - \tilde{\phi}(q) \tag{9}$$

$\tilde{\phi}(q)$ is the Fourier transform of ϕ on the lattice $\mathbb{Z}^d$. The function $\Delta(c)$ represents a gap in the spectrum (7) of self-consistent phonons. c_Λ is an order parameter measuring the mean square of the particle displacements from their equilibrium positions. The *stability condition* of the model is expressed by $\Omega_q^2(c) \geqslant 0$ for all $c \geqslant 0$ or equivalently by

$$a + 2W'(c) \geqslant 0 \qquad \text{for all } c \geqslant 0. \tag{10}$$

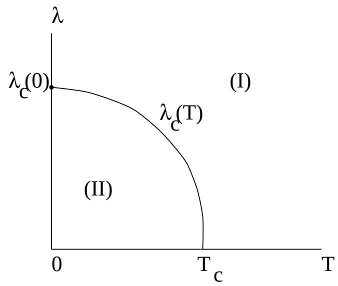

Figure 1. The phase diagram.

3. The phase diagram

The phase diagram can be obtained from the study of the gap equation (5) in the thermodynamic limit $\Lambda \to \mathbb{Z}^d$. It can then be written as

$$c = \rho + I_d(c, T, \lambda) \tag{11}$$

where

$$\rho = \lim_{\Lambda} \frac{1}{V} \frac{\lambda}{2\sqrt{\Delta(c)}} \coth \frac{\beta\lambda}{2} \sqrt{\Delta(c)} \tag{12}$$

$$I_d(c, T, \lambda) = \frac{\lambda}{(2\pi)^d} \int_{\mathcal{B}_d} \mathrm{d}^d q \, \frac{\coth(\frac{\beta\lambda}{2} \Omega_q(c))}{2\Omega_q(c)} \tag{13}$$

where $\mathcal{B}_d = \{q \in \mathbb{R}^d : |q_\alpha| \leqslant \pi\}$ is the first Brillouin zone.

Define the domain D as the set of those c which satisfy the stability condition. In [2] it is shown that $D = [c^*, \infty]$, where $c^* > 0$ is the solution of

$$c^* = I_d(c^*, T, \lambda).$$

We then have the following result.

Theorem 1.

(1) The equation

$$c^* = I_d(c^*, T, \lambda)$$

for fixed c^* defines a unique curve $\gamma = \lambda_c(T)$. This curve separates the phase diagram into two open domains, phases (I) and (II) (see figure 1).

(2) Let $\rho(T, \lambda) = \max\{0, c^* - I_d(c^*, T, \lambda)\}$; then

$$\begin{aligned} \rho(T, \lambda) &= 0 \qquad \text{if } (T, \lambda) \in \text{(I)} \cup \gamma \\ &> 0 \qquad \text{if } (T, \lambda) \in \text{(II)}. \end{aligned}$$

Proof.

(1) The proof is essentially the same as in [2], one only needs to check the concavity of the $T \to \lambda_c(T)$ curve. This can easily be done, and will yield that the concavity is independent of the particular form of the potential, or its Fourier transform $\tilde{\phi}(q)$.

(2) The proof of this part is completely the same as in [2]. □

A detailed discussion of the phase diagram can be found in [2]. We will restrict ourselves to the characterization of the two phases (I) and (II). In order to do this, note first that the Hamiltonian (1) has a Z^2 symmetry $Q_l \to -Q_l$ for $h = 0$, i.e.

$$\eta_\Lambda(Q_l) = 0.$$

The phase transition shows the spontaneous breaking of this symmetry, namely, in domain (II) there exist two extremal equilibrium states† η_+ and η_- such that

$$\eta_+(Q_l) = -\eta_-(Q_l) = \sqrt{\rho(T, \lambda)}.$$

4. Fluctuation operators and critical exponents

4.1. Fluctuation theory

In this section we repeat the essentials of the theory of fluctuations, needed for the calculation of the critical exponents, after which we proceed to calculate the critical exponents for observables P, Q and Q^2.

Consider $A_i = \tau_i(A)$ a copy of the local operator A, translated at the lattice point $i \in \mathbb{Z}^d$ by the automorphism τ_i. The fluctuation operator $F_\delta(A)$ in the ergodic translation-invariant state $\eta = \lim_\Lambda \eta_\Lambda$ on the algebra $\mathcal{A}$ of quasilocal observables is an unbounded operator on some Hilbert space, given by

$$F_\delta(A) = \lim_\Lambda \frac{1}{V^{\frac{1}{2}+\delta}} \sum_{i\in\Lambda} (A_i - \eta_\Lambda(A_i)). \tag{14}$$

The limit (14) is to be understood as a central limit. The exponent δ guarantees the existence of the fluctuation operator, when the following condition is satisfied

$$0 < \lim_\Lambda (F_\delta(A)^2) < \infty. \tag{15}$$

The critical exponent δ measures the deviation from the standard central limit (characterized by square-root behaviour). The following terminology is used in this respect. If $\delta = 0$ then the fluctuations are called *normal*. If $\delta > 0$ then the fluctuations are said to be *abnormal critical* and they are called *supernormal* or *squeezed* for $\delta < 0$.

The algebra of fluctuation operators is characterized by their commutators. For any two operators A and B, the commutator is

$$[F_{\delta_A}(A), F_{\delta_B}(B)] = \lim_\Lambda \frac{1}{V^{1+\delta_A+\delta_B}} \sum_{i\in\Lambda} [A_i, B_i]$$
$$= \begin{cases} \eta([A, B]) & \text{if } \delta_A + \delta_B = 0 \\ 0 & \text{if } \delta_A + \delta_B > 0 \\ \text{undefined} & \text{if } \delta_A + \delta_B < 0. \end{cases} \tag{16}$$

For $\eta([A, B]) \neq 0$, the non-vanishing commutator shows the quantum nature of the fluctuation operators.

For our model we will consider the algebra of observables generated by P, Q and Q^2. Their fluctuations are then given by

$$F_{\delta_Q}(Q) = \lim_\Lambda \frac{1}{V^{1/2+\delta_Q}} \sum_{l\in\Lambda} (Q_l - \eta_\Lambda(Q_l)) \tag{17}$$

† An explanation of all notions used in this paper can be found in [2], and a more thorough exposition on operator algebras and states can be found in [9].

$$F_{\delta_P}(P) = \lim_{\Lambda} \frac{1}{V^{1/2+\delta_P}} \sum_{l\in\Lambda} (P_l - \eta_\Lambda(P_l)) \tag{18}$$

$$F_{\delta_{Q^2}}(Q^2) = \lim_{\Lambda} \frac{1}{V^{1/2+\delta_{Q^2}}} \sum_{l\in\Lambda} (Q_l^2 - \eta_\Lambda(Q_l^2)). \tag{19}$$

Using the KMS equations, one can explicitly calculate the variances of these fluctuations. The following expressions are the result of this calculation:

$$\lim_{\Lambda} \eta_\Lambda(F_{\delta_Q}(Q)^2) = \lim_{\Lambda} \frac{1}{V^{2\delta_Q}} \frac{\lambda}{2\sqrt{\Delta(c_\Lambda)}} \coth\left(\frac{\beta\lambda}{2}\sqrt{\Delta(c_\Lambda)}\right) \tag{20}$$

$$\lim_{\Lambda} \eta_\Lambda(F_{\delta_P}(P)^2) = \lim_{\Lambda} \frac{1}{V^{2\delta_P}} \frac{\lambda m}{2}\sqrt{\Delta(c_\Lambda)} \coth\left(\frac{\beta\lambda}{2}\sqrt{\Delta(c_\Lambda)}\right) \tag{21}$$

$$\lim_{\Lambda} \eta_\Lambda(F_{\delta_{Q^2}}(Q^2)^2) = \lim_{\Lambda} \frac{1}{V^{1+2\delta_{Q^2}}} \frac{\lambda^2}{2\Delta(c_\Lambda)} \coth^2\left(\frac{\beta\lambda}{2}\sqrt{\Delta(c_\Lambda)}\right) + \sum_{q\neq 0} \frac{\lambda^2}{2\Omega_q(c)^2} \coth^2\left(\frac{\beta\lambda\Omega_q(c)}{2}\right). \tag{22}$$

The aim now is to find the exponents δ_Q, δ_P and δ_{Q^2} such that these variances are non-trivial. To accomplish this, it is necessary to understand the behaviour of the gap, as the thermodynamic limit is taken. This is the subject of section 4.2.

4.2. The form of the interactions, the gap equation

It turned out that the range of interactions does not influence the character of fluctuations if we are in the region of the phase diagram outside the critical line. If, however, we are *on* the critical line, the critical exponents are sensitive to the range of interactions [2, 3].

In this paper we consider short-range interactions but with anomalous low-momentum behaviour, namely

$$\tilde{\phi}(0) - \tilde{\phi}(q) \sim \sum_{i=1}^{d-1} q_i^2 + q_d^4. \tag{23}$$

Such a behaviour is exceptional (of codimension 1 in the space of parameters $\{\phi_k\}$), but can appear if one considers a one-parameter family of models.

The values of the δ-exponents we obtain from the analysis of equation (11) on the critical line. We have there $\rho = 0$, thus the asymptotic behaviour of the gap $\Delta(c_\Lambda(T_c, h = 0))$ is given by the condition

$$\lim_{\Lambda} \frac{1}{V} \frac{\lambda}{2\sqrt{\Delta(c_\Lambda)}} \coth \frac{\beta_c(\lambda)\lambda}{2}\sqrt{\Delta(c_\Lambda)} = 0. \tag{24}$$

We must distinguish two cases: $T_c(\lambda) > 0$; in this case equation (24) is equivalent to

$$\lim_{\Lambda} \frac{1}{V\beta_c(\lambda)\Delta(c_\Lambda)} = 0 \tag{25}$$

and the case $T_c(\lambda) = 0$, where equation (24) turns out to be

$$\lim_{\Lambda} \frac{\lambda}{2V\sqrt{\Delta(c_\Lambda)}} = 0. \tag{26}$$

In both cases, for $V \to \infty$ the gap $\Delta(c_\Lambda(T_c(\lambda), h = 0)) \approx V^{-\gamma}$ with $0 < \gamma < 1$. The exponent γ determines the values of δ_P, δ_Q and δ_{Q^2}. We obtain γ from the analysis of equation (5) for $h = 0$.

4.3. Case $T_c(\lambda) > 0$

4.3.1. Characteristics of the operator Q. Let us write the self-consistency equation (5) in the form

$$I + II + III = \frac{1}{V}\frac{\lambda}{2\sqrt{\Delta(c_\Lambda)}}\coth\frac{\beta_c(\lambda)\lambda}{2}\sqrt{\Delta(c_\Lambda)} \tag{27}$$

where

$$I = c_\Lambda - c^*$$
$$II = c^* - I_d(c_\Lambda, T_c(\lambda), \lambda)$$
$$III = I_d(c_\Lambda, T_c(\lambda), \lambda) - \frac{1}{V}\sum_{q\neq 0}\frac{\lambda}{2\Omega_q(c_\Lambda)}\coth\frac{\beta_c(\lambda)\lambda}{2}\Omega_q(c_\Lambda).$$

The analysis of equation (27) is performed analogously as in [2, 3]. The first term, I, from the left-hand side of (27) is proportional to Δ, because [2]

$$\frac{\Delta(c_\Lambda)}{2W''(c^*)} = (c_\Lambda - c^*) + \mathcal{O}(c_\Lambda - c^*).$$

The third term (III) behaves as

$$I_d(c_\Lambda, T_c, \lambda) - \frac{1}{V}\sum_{q\neq 0}\frac{\lambda}{2\Omega_q}\coth\frac{\beta_c\lambda}{2}\Omega_q = \mathcal{O}(\ln V^{-(d-2)/d}) \tag{28}$$

uniformly in $c_\Lambda \in D(c^*)$, where

$$I_d(c_\Lambda, T_c, \lambda) = \frac{1}{(2\pi)^d}\int_{\mathcal{B}^d}\mathrm{d}^d q\,\frac{\lambda}{2\Omega_q}\coth\frac{\beta\lambda}{2}\Omega_q.$$

Equality (28) was obtained by using a method developed in the appendix of [11].

Let us look at the second term:

$$II = c^* - I_d(c_\Lambda) = I_d(c^*) - I_d(c_\Lambda) = IIa + IIb \tag{29}$$

where

$$IIa = I_d^{(<\epsilon)}(c^*) - I_d^{(<\epsilon)}(c_\Lambda)$$
$$IIb = I_d^{(>\epsilon)}(c^*) - I_d^{(>\epsilon)}(c_\Lambda)$$

where the superscript $(<\epsilon)$ denotes the integral over a sphere of radius ϵ, and $(>\epsilon)$ denotes integral over the rest of the Brillouin zone.

Remark. What we need is an asymptotic behaviour of this equation for $\Delta \to 0$. It is singular in Δ (i.e. non-analytic), and this non-analytic behaviour is determined by the behaviour of the integrand in the neighbourhood of $q = 0$. The partition of the integration region as above was chosen as a matter of convenience.

The behaviour of $I^{(<\epsilon)}$ is determined by the lowest non-vanishing terms in the Taylor expansion of the denominator in the integrand. The asymptotic form of $I_d(c, T, \lambda)$ as $\Delta \to 0$ is calculated in the appendix (expression (42)). Dropping the constant term in this expression gives us the behaviour of IIa. Expression IIb has been calculated in exactly the same way as in [2], and it turns out that it is always proportional to Δ:

$$\{I_d^{(>\epsilon)}(c^*) - I_d^{(>\epsilon)}(c_\Lambda)\} = \frac{\Delta(c_\Lambda)}{2W''(c^*)}\partial_c I_d^{(>\epsilon)}(c'_\Lambda) + \mathcal{O}(c_\Lambda - c^*) \tag{30}$$

where $c'_\Lambda \in [c^*, c_\Lambda]$ (from the mean-value theorem).

We are looking for the asymptotic behaviour of Δ as a function of the volume V. It is determined from the equation [2]

$$[I + IIa + IIb + III]V\beta_c(\lambda)\Delta(c_\Lambda) = 1 \tag{31}$$

which has the solutions $\Delta \sim V^{-\gamma}$, where

$$\gamma = \begin{cases} \frac{4}{5} & \text{if } d = 3 \\ \frac{4}{7} & \text{if } d = 4 \\ \frac{1}{2} & \text{if } d \geqslant 5. \end{cases}$$

The calculation of δ_Q is now straightforward from equation (20); we have simply $\delta_Q = \frac{1}{2}\gamma$, or explicitly:

$$\delta_Q = \begin{cases} \frac{2}{5} & \text{if } d = 3 \\ \frac{2}{7} & \text{if } d = 4 \\ \frac{1}{4} & \text{if } d \geqslant 5. \end{cases} \tag{32}$$

4.3.2. Characteristics of the operator Q^2. For Q^2, it is necessary to analyse the behaviour of

$$\sum_{q\neq 0} \frac{1}{2\Omega_q(c)^2} \coth^2\left(\frac{\beta\lambda\Omega_q(c)}{2}\right)$$

when $\Delta \to 0$. This is done in much the same way as the analysis of the gap equation. We approximate the sum by an integral:

$$\begin{aligned} \eta_\Lambda(F_{\delta_{Q^2}}(Q^2)^2) = {} & \frac{1}{V^{1+2\delta_{Q^2}}} \frac{\lambda^2}{2\Delta(c_\Lambda)} \coth^2\left(\frac{\beta\lambda}{2}\sqrt{\Delta(c_\Lambda)}\right) \\ & + \frac{1}{V^{2\delta}}\left\{\frac{\lambda^2}{V}\sum_{q\neq 0}\frac{\coth^2(\frac{\beta\lambda\Omega_q(c)}{2})}{2\Omega_q(c)^2} - \int_{q\in\mathcal{B}} \mathrm{d}q\, \frac{\coth^2(\frac{\beta\lambda\Omega_q(c)}{2})}{2\Omega_q(c)^2}\right\} \\ & + \int_{q\in\mathcal{B}} \mathrm{d}q\, \frac{\lambda^2}{2\Omega_q(c)^2} \coth^2\left(\frac{\beta\lambda\Omega_q(c)}{2}\right). \end{aligned}$$

The analysis of this expression is done in exactly the same way as the analysis of the gap equation. Performing this analysis, one can see that the first term dominates the behaviour of the fluctuation as the gap disappears. The result then follows by using again the behaviour of the gap for large volumes

$$\delta_{Q^2} = \begin{cases} \frac{3}{10} & \text{if } d = 3 \\ \frac{1}{14} & \text{if } d = 4 \\ 0 & \text{if } d \geqslant 5. \end{cases} \tag{33}$$

4.3.3. Characteristics of the operator P. The result for P follows immediately from the behaviour of $\coth(x)$ for small x. It turns out that the momentum operator is *normal*.

4.4. Case $T_c(\lambda) = 0$

Here, we proceed exactly the same scheme as in the case of $T \neq 0$.

4.4.1. Characteristics of the operator Q. In this case equation (27) takes the form

$$\{c_\Lambda - c^*\} + \{c^* - I_d(c_\Lambda, 0, \lambda)\} + \left\{ I_d(c_\Lambda, 0, \lambda) - \frac{1}{V}\sum_{q\neq 0}\frac{\lambda}{2\Omega_q(c_\Lambda)} \right\} = \frac{\lambda}{2V\sqrt{\Delta(c_\Lambda)}} \qquad (34)$$

where

$$I_d(c_\Lambda, 0, \lambda_c(0)) = \frac{1}{(2\pi)^d}\int_{\mathcal{B}^d} \mathrm{d}^d q \, \frac{\lambda}{2\Omega_q(c_\Lambda)}. \qquad (35)$$

Using the second result from the appendix, (43), for obtaining the asymptotic dependence of Δ in the second term of equation (34), and then a method from [11, 2] for volume dependence of the third term in (34), and solving the analogue of the equation (31), we finally obtain the following dependence of Δ as a function of V: $\Delta \sim V^{-\gamma}$ with γ given by

$$\gamma = \begin{cases} \frac{4}{3} & \text{if } d = 2 \\ \frac{4}{5} & \text{if } d = 3 \\ \frac{2}{3} & \text{if } d = 4. \end{cases}$$

The calculation of δ_Q is straightforward; we simply have $\delta_Q = \frac{1}{4}\gamma$, or explicitly

$$\delta_Q = \begin{cases} \frac{1}{3} & \text{if } d = 2 \\ \frac{1}{5} & \text{if } d = 3 \\ \frac{1}{6} & \text{if } d = 4. \end{cases} \qquad (36)$$

4.4.2. Characteristics of the operator Q^2. The method used is identical to the case $T > 0$, and the result is

$$\delta_{Q^2} = \begin{cases} \frac{1}{24} & \text{if } d = 3 \\ 0 & \text{if } d \geqslant 4. \end{cases} \qquad (37)$$

4.4.3. Characteristics of the operator P. For P, we obtain that the momentum fluctuation operator has the critical exponent $\delta_P = -\delta_Q$ for all dimensions. This result follows from noting that for $T = 0$:

$$\eta_\Lambda(F_{\delta_P}(P)^2) = \frac{1}{V^{2\delta_P}}\frac{\lambda m}{2}\sqrt{\Delta(c_\Lambda)}$$

and

$$\eta_\Lambda(F_{\delta_Q}(Q)^2) = \frac{1}{V^{2\delta_Q}}\frac{\lambda}{\sqrt{\Delta(c_\Lambda)}}.$$

5. Conclusions

This paper can be considered as some continuation of investigations on the area of fluctuations in anharmonic crystal models. Other papers, which concerned similar circle of problems, are [2, 3].

This circle of problems can be considered as part of a broader programme. Namely, to see how a general theory of quantum fluctuations works in concrete physical models. One can mention here the following subject: Bose–Einstein gas [13, 14].

The concrete aim of this paper was to check in which manner the effect of the asymmetry in the phonon spectrum manifests itself. We assumed the following form of the phonon spectrum for a d-dimensional model: in one direction it has quartic low-momentum asymptotics, and in the remaining directions the spectrum is ordinary quadratic. In the paper we examined the details of the behaviour of the model (especially on the critical line) along the lines of [2]. The following has been established.

- The phase diagram of the model remained unchanged, compared with the symmetric model [2]. Moreover, the character of fluctuations (i.e. their normality, ab- and super-normality) has not changed in the different parts of the phase diagram.
- What *has* changed is the behaviour on the critical line, measured quantitatively by the δ exponent. It was always larger in comparison with the symmetric model, independently of dimension, and for both $T > 0$ and $T = 0$. In more physical terms, the fluctuations are always stronger in the (our) case of asymmetric anharmonicity. (It should be stressed that if we have the *asymmetric* form of the phonon spectrum, but purely quadratic: $\tilde{\phi}(0) - \tilde{\phi}(q) \sim \sum_{i=1}^{d} a_i q_i^2$, then the critical exponents are *independent* of the values of a_i, provided all $a_i > 0$.)
- It has been established that the fluctuations do not form a Lie algebra, different from the CCR algebra, as described in [15]. This follows immediately from the values of δ for P, Q and Q^2.

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Appendix. A representative calculation

The asymptotic behaviour of the integrals appearing in the study of the gap equation can be studied by using a scaling argument. In this appendix we present, as an example, the calculation of the behaviour of the following integral when $\Delta \to 0$:

$$I_d(c, T, \lambda) = \int_{\mathcal{B}} \mathrm{d}^d q \, \frac{1}{\Omega_q(c)} \coth\left(\frac{\beta\lambda}{2}\Omega_q(c)\right) \tag{38}$$

for $T > 0$. The divergence of this integral is dominated by the behaviour of the integrand at distances close to the origin. We therefore split the Brillouin zone in a part close to the origin, say $|q| < \epsilon$, and the rest. Then (38) becomes

$$\int_{|q|<\epsilon} \mathrm{d}^d q \, \frac{1}{\Omega_q(c)} \coth\left(\frac{\beta\lambda}{2}\Omega_q(c)\right) + \int_{|q|>\epsilon} \mathrm{d}^d q \, \frac{1}{\Omega_q(c)} \coth\left(\frac{\beta\lambda}{2}\Omega_q(c)\right).$$

The integral where $|q| > \epsilon$ is non-divergent for $\Delta \to 0$, so we can consider the region close to the origin, and approximate $\coth(x) \sim \frac{1}{x}$ for small x. Thus, the integral becomes

$$\frac{2}{\beta\lambda} \int_{|q|<\epsilon} \mathrm{d}^d q \, \frac{1}{\Omega_q^2(c)} = \frac{2}{\beta\lambda} \int_{|q|<\epsilon} \mathrm{d}^d q \, \frac{1}{\Delta + \tilde{\phi}(0) - \tilde{\phi}(q)}. \tag{39}$$

We must calculate the behaviour as $\Delta \to 0$ of the following integral:

$$\underset{\mathcal{U}}{\int \cdots \int} \mathrm{d}x_1 \ldots \mathrm{d}x_d \, \frac{1}{\Delta + \sum_{i=1}^{d-1} x_i^2 + x_d^4} \tag{40}$$

(d denotes the dimension). Both integrals: (39) and (40), have the same behaviour as functions of Δ. It is not necessary to specify explicitly the form of the integration domain $\mathcal{U}$. We demand only that $\mathcal{U}$ should be an open neighbourhood of zero. (Its size is of order ϵ.) We substitute

$$\begin{cases} y_i = x_i & i < d \\ y_d = x_d^2 \end{cases} \tag{41}$$

then we obtain

$$\int_{\tilde{\mathcal{U}}} \cdots \int \mathrm{d}y_1 \ldots \mathrm{d}y_d \, \frac{1}{2\sqrt{y_d}} \frac{1}{\Delta + \sum_{i=1}^d y_i^2}$$

($\tilde{\mathcal{U}}$ is the domain $\mathcal{U}$ in new variables). We switch to polar coordinates and integrate over some ball of radius R^2, centred at zero and contained in $\tilde{\mathcal{U}}$. We obtain:

$$\int_0^{R^2} \mathrm{d}r \int_\Omega \cdots \int \mathrm{d}^{d-1}\Omega \, \frac{r^{d-1}}{(\Delta + r^2)\sqrt{rf(\Omega)}}$$

where Ω denotes the space angles. Performing integration over the space angles (the result is finite, because the singularities of the integrand are integrable), leaves us with the integral

$$S_d \int_0^{R^2} \mathrm{d}r \, \frac{r^{d-3/2}}{(\Delta + r^2)}$$

(S_d is some constant depending on the dimension). Now, we perform the substitution $r = \sqrt{\Delta}\rho^2$ and obtain

$$2S_d \Delta^{d/2-5/4} \int_0^{R/\Delta^{1/4}} \mathrm{d}\rho \, \frac{\rho^{2d-3}}{(1+\rho^4)}.$$

In the sequel, we will consider the integrals in dimensions of importance for us.

• $d = 3$. Consider first:

$$I_3 \sim \Delta^{1/4} \int_0^{R/\Delta^{1/4}} \mathrm{d}\rho \, \frac{\rho^4}{(1+\rho^4)} = \Delta^{1/4}\left(\int_0^{R/\Delta^{1/4}} \mathrm{d}\rho - \int_0^{R/\Delta^{1/4}} \frac{\mathrm{d}\rho}{1+\rho^4} \right)$$
$$= \Delta^{1/4}(R/\Delta^{1/4} + J_3 + \mathcal{O}(\Delta^{3/4}))$$

where $J_3 = \int_0^\infty \frac{\mathrm{d}\rho}{1+\rho^4}$. So, we finally obtain

$$I_3 \sim C_3 + C_3' \Delta^{1/4}.$$

It should be stressed that the constant C_3' is *independent* of the choice of the $\mathcal{U}$ set.

• $d = 4$. We have:

$$I_4 \sim \Delta^{3/4} \int_0^{R/\Delta^{1/4}} \mathrm{d}\rho \, \frac{\rho^6}{(1+\rho^4)} = \Delta^{3/4}\left(\int_0^{R/\Delta^{1/4}} \rho^2 \, \mathrm{d}\rho - \int_0^{R/\Delta^{1/4}} \frac{\rho^2 \mathrm{d}\rho}{1+\rho^4} \right)$$
$$= \Delta^{3/4}(R^3\Delta^{-3/4}/3 + J_4 + \mathcal{O}(\Delta^{1/4}))$$

where $J_4 = \int_0^\infty \frac{\rho^2\,\mathrm{d}\rho}{1+\rho^4}$. So, the final result is

$$I_4 \sim C_4 + C_4' \Delta^{3/4}.$$

• $d = 5$. By identical arguments as before

$$I_5 \sim R^5/5 + R\Delta + J_3\Delta^{5/4} + \Delta^{5/4}\mathcal{O}(\Delta^{3/4})$$

so we have as the dominant terms

$$I_5 \sim C_5 + C_5' \Delta.$$

It is easy to see that we have the same Δ-dependence for dimensions higher than 5.

We can therefore conclude that integral (38) has the following behaviour:

$$I_d(c, T, \lambda) \sim C_d + C_d' \Delta^\theta \qquad \text{where } \theta = \begin{cases} \frac{1}{4} & \text{if } d = 3 \\ \frac{3}{4} & \text{if } d = 4 \\ 1 & \text{if } d \geqslant 5 \end{cases} \tag{42}$$

(remember $T > 0$!). Arguing along the same lines, one comes to the conclusion that for zero temperature

$$I_d(c, 0, \lambda) = \int_{\mathcal{B}} \mathrm{d}^d q \, \frac{1}{\Omega_q(c)} \sim \tilde{C}_d + \tilde{C}_d' \Delta^\tau \tag{43}$$

where

$$\tau = \begin{cases} \frac{1}{4} & \text{if } d = 2 \\ \frac{3}{4} & \text{if } d = 3 \\ 1 & \text{if } d \geqslant 4. \end{cases}$$

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