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# Phase Transitions and Algebra of Fluctuation Operators in an Exactly Soluble Model of a Quantum Anharmonic Crystal

**A. Verbeure[1] and V. A. Zagrebnov[1,2]**

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A complete description of the fluctuation operator algebra is given for a quantum crystal showing displacement structural phase transitions. In the one-phase region, the fluctuations are normal and its algebra is non-Abelian. In the two-phase region and on the critical line ($T_c > 0$) the momentum fluctuation is normal, the displacement is critical, and the algebra is Abelian; at $T_c = 0$ (quantum phase transition) this algebra is non-Abelian with abnormal displacement and supernormal (squeezed) momentum fluctuation operators, both being dimension dependent.

**KEY WORDS:** Algebra of fluctuation operators; abnormal and supernormal (squeezed) fluctuations; quantum phase transition.

## 1. INTRODUCTION

In this paper we mainly turn our attention to critical fluctuations, i.e., to fluctuations on the critical line of the phase diagram. In the physics of collective phenomena it belongs to the standard wisdom that critical fluctuations wash out quantum effects. The intuitive heuristic argument for this is that critical fluctuations are manifestations of long-range correlations and that quantum effects are hidden by the long-range correlations in the critical region. The fluctuations behave classically (see, e.g., ref. 1).

However, from the experimental side there is a continuous interest in the detection of quantum phenomena in critical regions where long-range

[1] Instituut voor Theoretische Fysica, Katholieke Universiteit Leuven, B-3001 Leuven, Belgium.
[2] On leave of absence from Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna 141980, CIS (Russia).

correlations show up. One observes great activity in the search for these effects in perovskite crystal structures like $SrTiO_3$ and $KTaO_3$. For recent measurements indicating a novel quantum phase transition see, e.g., ref. 2. What seems to be clear is that there exists experimental evidence for the existence of typical quantum effects observed in critical fluctuations, challenging the above intuitive heuristic argument, which seems to be too crude to explain these experimental results. We argue this point with rigor on the basis of the study of a model.

Recently[3–5] a theory was developed that is suitable to handle the joint description of two and more macroscopic equilibrium fluctuations. Another relevant point is that the notion of a fluctuation as an observable and operator was introduced. The work is done for genuine quantum systems. The main outcome is that the set of macroscopic fluctuations can be jointly described in a canonical way by a *boson field*. Due to the coarse graining of the central limit theorem, the fluctuations of two or more noncommuting local observables can commute or not. If they all commute, no quantum effects in this sense are observed—on the level of the fluctuations. They are described by a classical field and one speaks about *classical fluctuations*. In case the set of fluctuation observables is noncommutative, one speaks about *quatum fluctuations*. Clearly, in a classical system one never observes quantum fluctuations.

Ellis and Newman[6] showed that classical Curie–Weiss models at the thermal critical point $T_c$ have critical abnormal fluctuations if one takes *simultaneously* the infinite limit for the size of the system and for the number of random variables.

Recently[7] this question has been studied for quantum mean-field models showing also critical behavior. It was observed that the critical fluctuations are purely classical in agreement with the widespread belief.

Here we consider a model invented to study displacive structural phase transitions with general anharmonicity.[8,9] We consider a $d$-dimensional square lattice $\mathbb{Z}^d$; at each lattice point $l \in \mathbb{Z}^d$ we associate a quantum particle with mass $m$, position $Q_l \in \mathbb{R}^1$, and momentum $P_l$. The local Hamiltonian $H_\Lambda$ for any finite subset $\Lambda$ of $\mathbb{Z}^d$ is given by

$$\begin{aligned} H_\Lambda(h) = \sum_{l \in \Lambda} \frac{P_l^2}{2m} + \frac{1}{4} \sum_{l, l' \in \Lambda} \phi_{l-l'}(Q_l - Q_{l'})^2 \\ + \frac{a}{2} \sum_{l \in \Lambda} Q_l^2 + |\Lambda| \, W\left( \frac{1}{|\Lambda|} \sum_{l \in \Lambda} Q_l^2 \right) - h \sum_{l \in \Lambda} Q_l \end{aligned} \tag{1.1}$$

The first two terms represent the Debye phonon approximation; the third term describes the stabilization of the lattice and creates a gap in the phonon spectrum for $a > 0$. A typical example of the potential $W$ is $W(x) = (b/2)\exp(-\eta x)$; $b, \eta > 0$ and $b$ sufficiently large.[8]

This model shows two types of phase transitions. On one hand, it has the usual mean-field phase transition controlled by the parameter temperature, which has been studied carefully before.[9,10] On the other hand, at $T = 0$, we exhibit a transition of a pure quantum nature controlled by the quantum parameter $\lambda = \hbar/\sqrt{m}$.

In this model we compute the fluctuations in each of the critical points $T_c$ and $\lambda_c$ along the lines of ref. 11. Our calculations are guided by the ideas developed recently by one of us.[3-5] In order to make the idea clear without entering into the technical details, consider the square lattice $\mathbb{Z}^d$ quantum system and $A_i$, $B_j$ copies of local observable operators $A$ and $B$ at the sites $i, j \in \mathbb{Z}^d$. In refs. 3 and 4 it is proved that one can given a mathematical meaning to the limits

$$F_0(A) = \lim_V \frac{1}{\sqrt{V}} \sum_{i \in \Lambda} (A_i - \langle A \rangle); \qquad \Lambda \in \mathbb{Z}^d, \quad V = |\Lambda| \tag{1.2}$$

in the sense of a central limit theorem, i.e., with respect to a space translation-invariant state $\langle \cdot \rangle$ which might be a thermal state or a ground state.

One proves that for any $A$ the limit $F_0(A)$ is an unbounded operator. It is called the *fluctuation operator* of $A$ in the state $\langle \cdot \rangle$.

One can compute the commutator of two fluctuation operators in the follows sense:

$$\begin{aligned}[F_0(A), F_0(B)] &= \lim_N \left[\frac{1}{\sqrt{V}} \sum_{i \in \Lambda} A_i - \langle A \rangle, \frac{1}{\sqrt{V}} \sum_{j \in \Lambda} B_j - \langle B \rangle\right] \\ &= \lim_V \frac{1}{V} \sum_{i \in \Lambda} [A_i, B_i]\end{aligned} \tag{1.3}$$

The right-hand side of this equality is a mean average, equal to a constant, of the expectation value $\langle [A, B] \rangle$ if $\langle \cdot \rangle$ is an ergodic state. If $\langle [A, B] \rangle \neq 0$, the commutator (1.3) yields a nontrivial canonical commutation relation between two fluctuation operators:

$$[F_0(A), F_0(B)] = \langle [A, B] \rangle \mathbb{1} \tag{1.4}$$

indicating the quantum character of these fluctuations.

The *normality* of the fluctuation defined by (1.2) manifests itself in the factor $V^{-1/2}$ in front of the sum.

Our model results are about fluctuation operators for equilibrium and ground states at the critical points. The results include the following points.

(i) As in ref. 11, one finds at the critical points fluctuation operators $F_\delta$ of the type (1.2), but carying a normalization $V^{-1/2-\delta}$, $\delta \in (-1/2, 1/2)$, showing a deviation from the standard square root; the parameter $\delta$ (*critical exponent*) measures the degree of *criticality* of the corresponding fluctuation operator.

(ii) In the ground state we exhibit a "pure quantum" transition and there exist a pair of local operators $A$ and $B$ in the model such that the fluctuation of $A$ is of the type $F_\delta(A)$ with $\delta > 0$ and the fluctuation of $B$ is of the type $F_{-\delta}(B)$. Usually one calls fluctuations $F_\delta(A)$ with $\delta > 0$ *abnormal critical* fluctuations. The new type $F_{-\delta}(B)$, $\delta > 0$, will be called *supernormal* (*squeezed*) *critical* fluctuations.

(iii) Moreover, the critical fluctuation operators $F_\delta(A)$ and $F_{-\delta}(B)$ satisfy the following canonical commutation relation:

$$[F_\delta(A), F_{-\delta}(B)] = \langle [A, B] \rangle \mathbb{1} \neq 0 \tag{1.5}$$

generalizing (1.4), and what is even more interesting, putting forward unambiguously the *quantum nature* of critical fluctuations.

(iv) The dimension dependence of the critical parameter $\delta$ can be explicitly calculated.

This paper is organized as follows. In Section 2, we give a complete description of the thermodynamics or the phase diagram of the model (1.1).

In Section 3, we give more detailed information about the model by constructing explicitly its equilibrium and ground states. Much attention is given to the phenomenon of spontaneous symmetry breaking. This is necessary in order to understand the nature of the phase transitions present.

The bulk of our contribution is given in Section 4, where we give complete results about the momentum and displacement fluctuation operators in all points of the phase diagram. We distinguish *four* regions. The *first* is the one-phase region (except the critical line), where all fluctuations are *normal* and the algebra of fluctuation operators is *non-Abelian.*

In the *two-phase* region, the momentum fluctuation is *normal,* while the displacement fluctuation is *abnormal critical* with a critical exponent which depends explicitly on the boundary condition. The algebra of fluctuation operators is *Abelian.*

The *third* region which we can consider is the critical line except the point $T_c = 0$. Here we prove rigorously that the momentum fluctuation is *normal* and the displacement fluctuation *abnormal critical.* We find the exact values of the critical exponents, they do not depend on the boundary conditions, but they depend on the dimensionality of the system. Here also the algebra of fluctuation operators is *Abelian.*

Finally, at the *critical point* $T_c = 0$, we find a pure quantum transition at a critical value $\lambda_c$ of the quantum parameter $\lambda = \hbar/\sqrt{m}$. At this point we compute also the dimension-dependent critical exponents of momentum and displacement fluctuations. We prove that these fluctuation operators generate a *non-Abelian* algebra, putting in evidence the quantum character at criticality. The displacement fluctuation is *abnormal critical,* but the momentum fluctuation is *squeezing.* Also at this point, the critical exponents are independent of the boundary conditions.

## 2. MODEL AND PHASE DIAGRAM

First we introduce the model. Let $\mathscr{H} = L^2(\mathbb{R}^1)$; $\mathbb{Z}^d$ is the $d$-dimensional square lattice with local structure; denote by $\mathscr{D}(\mathbb{Z}^d)$ the directed set of finite subsets of $\mathbb{Z}^d$, where the direction is the inclusion. With each $\Lambda \in \mathscr{D}(\mathbb{Z}^d)$ we associate the local algebra $\mathscr{B}_l$, $l \in \Lambda$, of operators on $\mathscr{H}$ generated by the operators $R(P)\, f(Q)$, where $R$ runs through the polynomials and $f$ is in $C_0^\infty$; $Q$ and $P$ stand for the usual canonical observables of multiplication and differentiation (i.e., $[Q, P] = i\hbar$).

For each $\Lambda \in \mathscr{D}(\mathbb{Z}^d)$, denote the tensor product $\mathscr{B}_\Lambda = \bigotimes_{l \in \Lambda} \mathscr{B}_l$; the algebra of local observables is then the union $\mathscr{A} = \bigcup_\Lambda \mathscr{B}_\Lambda$.

The model Hamiltonian for each $\Lambda \in \mathscr{D}(\mathbb{Z}^d)$, with $V = |\Lambda|$ the volume of $\Lambda$, is given by

$$H_\Lambda = T_\Lambda + VW\left(\frac{1}{V} \sum_{l \in \Lambda} Q_l^2\right) \tag{2.1}$$

where [cf. (1.1)]

$$T_\Lambda = \frac{1}{2m} \sum_{l \in \Lambda} P_l^2 + \frac{a}{2} \sum_{l \in \Lambda} Q_l^2 + \frac{1}{4} \sum_{l, l' \in \Lambda} \phi_{ll'} (Q_l - Q_{l'})^2 \tag{2.2}$$

$Q_l$ and $P_l$ are the displacement and momentum of a particle with mass $m$ at the site $l \in \mathbb{Z}^d$; the potential is supposed to be translation invariant ($\phi_{ll'} = \phi_{l-l'}$) and of finite range; the $W$ term in (2.1) is meant to include the anharmonicity. To describe a displacive structural phase transition, we take a double-well potential form for the $a$ term + $W$ term: for example, $a > 0$ and the function $W(x) = (b/2) \exp(-\eta x)$ with $b, \eta > 0$ and $b$ sufficiently large to destabilize the $a$ term.[8,9] Another example is $a < 0$ (one-site instability) and $W(x) = \frac{1}{2} b x^2$, $b > 0$.[10] Hence, now the $W$ term stabilizes the lattice. This *polynomial* choice of anharmonicity is known as the

$\varphi^4$-model for structural phase transitions. The particular choice of the function $W$ will be unimportant for the considerations below if $W$ satisfies some general conditions.[9] The substitution of $Q_l^2$ by the arithmetic mean over $\Lambda$ is an *ansatz* corresponding to the concept of the *self-consistent-phonons* (see, e.g., ref. 12).

The model (2.1) 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 Appendix). Take the hypercubic subset $\Lambda \subset \mathbb{Z}^d$ wrapped according to the periodic boundary conditions:

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

Then $V = \prod_{d=1}^{d} N_\alpha$ and the dual volume $\Lambda^*$ is given by

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

The free energy density for this model is given by

$$f(T, h=0) = \lim_{\Lambda} \left\{ \frac{1}{\beta V} \sum_{q \in \Lambda^*} \ln[2 \operatorname{sh} \beta\lambda\Omega_q(c_\Lambda)] + W(c_\Lambda) - c_\Lambda W'(c_\Lambda) \right\} \tag{2.3}$$

where $c_\Lambda$ is a solution for $c$ of the self-consistency equation

$$c = \left\langle \frac{1}{V} \sum_{l \in \Lambda} Q_l^2 \right\rangle_{H_\Lambda(c, h=0)} = \frac{1}{V} \sum_{q \in \Lambda^*} \frac{\lambda}{2\Omega_q(c)} \coth \frac{\beta\lambda}{2} \Omega_q(c) \tag{2.4}$$

see Appendix, Eq. (A15).

Here $\beta = 1/kT$ and

$$\lambda = \frac{\hbar}{\sqrt{m}} \tag{2.5}$$

$$\Omega_q^2(c) = \omega_q^2 + \Delta(c) \tag{2.6}$$

$$\Delta(c) = a + 2W'(c) \tag{2.7}$$

$$\omega_q^2 = \tilde{\phi}(0) - \tilde{\phi}(q) \tag{2.8}$$

$\tilde{\phi}$ is the Fourier transform of $\phi$ on the lattice $\mathbb{Z}^d$. The *stability condition* of the model is expressed by $\Omega_q^2(c) \geqslant 0$ for all $c \geqslant 0$ or equivalently[9] by

$$a + 2W'(c) \geqslant 0 \qquad \text{for all} \quad c \geqslant 0 \tag{2.9}$$

Clearly $c_\Lambda$ is an order parameter measuring the mean square of the particle displacements from their equilibrium positions [see (A.15)]; $\Delta(c)$ is a gap in the spectrum (2.6) of collective excitations, the phonons.

The study of the phase diagram of the model amounts to the study of the solutions of Eq. (2.4) in the thermodynamic limit $\Lambda \to \mathbb{Z}^d$. Equation (2.4) reads then

$$c = \rho + I_d(c, T, \lambda) \tag{2.10}$$

where

$$\rho = \lim_{\Lambda} \frac{1}{V} \frac{\lambda}{2[\Delta(c)]^{1/2}} \coth \frac{\beta\lambda}{2} [\Delta(c)]^{1/2} \tag{2.11}$$

$$I_d(c, T, \lambda) = \frac{\lambda}{(2\pi)^d} \int_{\mathfrak{B}_d} d^d q \, \frac{\coth(\beta\lambda/2)\, \Omega_q(c)}{2\Omega_q(c)} \tag{2.12}$$

Here $\mathfrak{B}_d = \{q \in \mathbb{R}^d \colon |q_\alpha| \leqslant \pi\}$ is the first Brillouin zone. For fixed $T > 0$ and $\lambda$, the integral (2.12) is finite if $d \geqslant 3$ and $c$ satisfies the stability condition (2.9). For $T = 0$ and fixed $\lambda$, the integral (2.12) is finite if $d \geqslant 2$.

Let us introduce the domain $D$ of $c$ satisfying the stability condition (2.9). Define $c^*$ as follows:

$$c^* = \inf\{c \mid c \geqslant 0;\ \Delta(c) \geqslant 0\} \tag{2.13}$$

Then for a particular choice of anharmonicity, as $W(x) = b/2 \exp(-\eta x)$, one gets $c^* = \max\{0, \eta^{-1} \ln b\eta/a\}$.

Because $W' < 0$, the infimum is attained at $c^*$ such that $\Delta(c^*) = 0$. Hence the domain for the order parameter $c = c(T, \lambda)$ as a solution of (2.10) is the interval $D = [c^*, \infty)$.

Remark also that the value of $c^*$ depends on the form of the harmonic and anharmonic parts of the one-particle potential; hence, changing the characteristics of the potential changes the value of $c^*$ for the domain $D$. Also, fixing the shape of the potential fixes $c^*$ or the stability domain $D$ for $c$. In fact, the requirement of the double-well form of the potential means already that $c^* > 0$.

**Proposition 2.1.** (i) The equation

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

for fixed $c^*$ defines a unique curve $\lambda_c(T)$ expressed as a function of $T$, or $T_c(\lambda)$ expressed as a function of $\lambda$.

This curve separates the $(T, \lambda)$ plane into two parts indicated by phase (I) and phase (II); see Fig. 1.

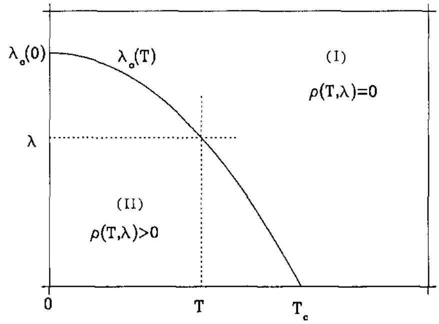


Fig. 1. Phase diagram of the model (2.1).

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

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

In other words, in the phase region (I) one has a solution of (2.10) with $\rho = 0$ and in phase region (II) one has $\rho > 0$.

*Proof.* (i) From the explicit form of the integral $I_d$ in (2.12) one gets a solution $\lambda_c(0) < \infty$ of the equation

$$I_d(c^*, 0, \lambda_c(0)) = c^*$$

and also a solution $T_c(0) < \infty$ from the equation

$$I_d(c^*, T_c(0), 0) = c^*$$

Computing the first and second derivatives of $T \to I_d(c^*, T, \lambda_c(T))$ yields that $T \to \lambda_c(T)$ is concave, as indicated in Fig. 1, separating the $(T, \lambda)$ plane into the regions (I) and (II).

(ii) Remark that the function $I_d(c^*, T, \lambda)$ is monotonically increasing independently in the variables $T$ and $\lambda$. Therefore

$$\begin{aligned} I_d(c^*, T, \lambda) &> c^* \qquad \text{iff} \quad (T, \lambda) \in (\mathrm{I}) \\ I_d(c^*, T, \lambda) &< c^* \qquad \text{iff} \quad (T, \lambda) \in (\mathrm{II}) \\ I_d(c^*, T, \lambda) &= c^* \qquad \text{iff} \quad \lambda = \lambda_c(T) \end{aligned}$$

Remark that the function $c \to c - I_d(c, T, \lambda)$ is monotonically increasing and

$$\min_{c \in D}(c - I_d(c, T, \lambda)) = c^* - I_d(c^*, T, \lambda)$$

Therefore

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

is given by

$$\rho(T, \lambda) = 0 \quad \text{if} \quad (T, \lambda) \in (\mathrm{I}) \cup \partial(\mathrm{I})$$

$$\rho(T, \lambda) > 0 \quad \text{if} \quad (T, \lambda) \in (\mathrm{II})$$

Furthermore, remark that $c \to \sim I_d(c, T, \lambda)$ is monotonically decreasing (see Fig. 2). Therefore Eq. (2.10) always has a solution for $c(T, \lambda)$, with $\rho = 0$ if $(T, \lambda) \in (\mathrm{I}) \cup \partial(\mathrm{I})$ and $\rho > 0$ if $(T, \lambda) \in (\mathrm{II})$. ∎

Coming back to Fig. 1, and looking along a vertical ($T = \text{const}$) dotted line in the figure, if $\lambda < \lambda_c(T)$, then $\rho > 0$. Increasing $\lambda$ across the critical line $\lambda_c(T)$, we have a phase transition going from a regime $\rho > 0$ to a regime $\rho = 0$. We observe a phase transition driven by the quantum parameter $\lambda$ of (2.5) for each temperature $T < T_c(0)$.

As remarked above, changing the shape of the double-well potential changes the value of $c^* > 0$. One obtains the same type of phase diagram in the variables $(c^*, T)$ as in the variables $(\lambda, T)$.

The other, well-known, phase transition in this model which is driven by the temperature is observed in the phase diagram of Fig. 1 by looking along a horizontal ($\lambda = \text{const}$) dotted line. If $\lambda < \lambda_c(0)$, one is in the regime $\rho > 0$ for low temperatures $T$, and with increasing $T$ one crosses the phase line $\lambda_c(T)$ before entering the phase $\rho = 0$. Note that if one fixed $\lambda > \lambda_c(0)$, then upon decreasing the temperature, one will never cross the critical line, which means that for large values of the quantum parameter $\lambda$, the temperature-driven phase transition is *suppressed* by quantum tunneling or *quantum fluctuations*. Note also that the *classical limit* of the model is obtained in the limit $\lambda \to 0$, such that $T_c(0)$ is the critical temperature of the classical model.

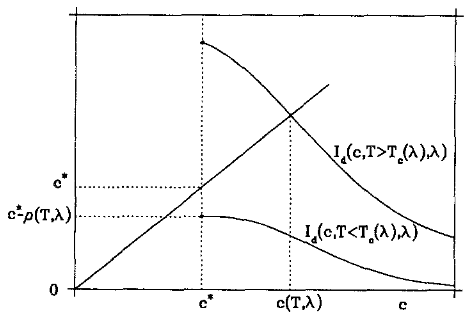


Fig. 2. Graphical solution of the equation (2.10)

## 3. GROUND STATE, EQUILIBRIUM STATES

In Section 2 we introduced the model and the algebra of local observables of the system: $\mathscr{A} = \bigcup_\Lambda \mathscr{B}_\Lambda$, where $\mathscr{B}_\Lambda$ is generated by the algebra of $Q_l$ and $P_l$, $l \in \Lambda$, the canonical position and momentum operators.

In general a state of our system is any positive, linear, normalized form $\omega$ on $\mathscr{A}$.

For any $a \in \mathbb{Z}^d$, denote by $\tau_a$ the lattice translation $*$-automorphism defined on $\mathscr{A}$ by

$$\tau_a Q_l = Q_{l+a}, \qquad \tau_a P_l = P_{l+a}$$

A state $\omega$ is called lattice translation invariant if $\omega \cdot \tau_a = \omega$ for all $a \in \mathbb{Z}^d$; $\omega$ is called ergodic or extremal translation invariant if furthermore

$$\lim_{|a| \to \infty} \omega(A \tau_a B) = \omega(A)\,\omega(B)$$

for all $A, B \in \mathscr{A}$.

We are interested in the ergodic equilibrium and ground states of the system determined by the model Hamiltonian (2.1), to which we add an external field term [cf. (1.1)]:

$$H_\Lambda(h) = T_\Lambda + VW\left(\frac{1}{V} \sum_{l \in \Lambda} Q_l^2\right) - h \sum_{l \in \Lambda} Q_l \tag{3.1}$$

The external field $h$ plays the role of a boundary condition. Finally, we will be interested in the states obtained in the limit $h \to 0$ in a specific way, in order to eliminate all degeneracies.

For the purpose of this paper it is useful to characterize equilibrium and ground states by means of correlation inequalities.[13]

For $T > 0$ ($\beta < \infty$), a state $\omega$ is an equilibrium state if for all $A \in \mathscr{A}$ one has

$$\beta\omega(A^*\delta_h(A)) \geqslant \omega(A^*A) \ln \frac{\omega(A^*A)}{\omega(AA^*)} \tag{3.2}$$

and for $T = 0$, $\omega$ is a ground state if for all $A \in \mathscr{A}$ one has

$$\omega(A^*\delta_h(A)) \geqslant 0 \tag{3.3}$$

where the derivation $\delta_h$ is weakly defined by: $A, B \in \mathscr{A}$, then

$$\omega(A\delta_h(B)) = \lim_\Lambda \omega(A[H_\Lambda(h), B]) \tag{3.4}$$

In writing these equilibrium conditions, we implicitly assume that we are looking at those solutions $\omega$ for which these limits exist.

Before going on, already at this point we want to indicate that the characterizations (3.2) and (3.3) make it clear that the equilibrium and ground states are essentially determined by the derivation $\delta_h$ of (3.4), i.e., by the commutator with the Hamiltonian.

Furthermore, the Hamiltonian (3.1) is lattice translation invariant. Therefore we will only look for solutions $\omega$ of (3.2) and (3.3) which are translation invariant. In other words, we assume that there is no spontaneous breaking of this translation symmetry. While we are unable to show this property, we strongly believe that this is not really a condition. Translation-invariant states have the property that they can be decomposed into ergodic states. This means that there exists a probability measure, denoted by $v$, with support on the set $\mathscr{E}$ of ergodic states such that (ref. 14, Chapter 4)

$$\omega(\cdot)=\int_{\mathscr{E}} dv(\eta)\,\eta(\cdot)$$

By this formula and because of the convexity of both sides of (3.2) and (3.3), it is sufficient to consider the solutions $\eta\in\mathscr{E}$ of the inequalities

$$\beta\eta(A^*\delta_h(A))\geqslant\eta(A^*A)\ln\frac{\eta(A^*A)}{\eta(AA^*)} \tag{3.5}$$

$$\eta(A^*\delta_h(A))\geqslant 0 \tag{3.6}$$

The main property of these ergodic states $\eta\in\mathscr{E}$ is the existence of the ergodic means; for all local operators $A$, $B$, $C\in\mathscr{A}$ one has

$$\lim_{\Lambda}\eta\left(A\left(\frac{1}{V}\sum_{x\in\Lambda}\tau_x B\right)C\right)=\eta(AC)\,\eta(B)$$

i.e.,

$$\eta\text{-weak-}\lim_{\Lambda}\frac{1}{V}\sum_{x\in\Lambda}\tau_x B=\eta(B)$$

In particular, take $B=Q_0^2$; then

$$\eta\text{-weak-}\lim_{\Lambda}\frac{1}{V}\sum_{l\in\Lambda}Q_l^2=\eta(Q_0^2) \tag{3.7}$$

We use this property in order to prove that, if one is interested only in the ergodic solutions, one can work with an equivalent system, defined by an effective Hamiltonian $H_\Lambda^\eta(h)$ given by the following result.

**Proposition 3.1.** For all $A, B \in \mathscr{A}$, we have

$$\eta(A\delta_h^\eta(B)) = \lim_{\Lambda} \eta(A[H_\Lambda^\eta(h), B])$$

where

$$H_\Lambda^\eta(h) = \sum_{l \in \Lambda} \frac{P_l^2}{2m} + \frac{1}{4} \sum_{l, l' \in \Lambda} \Phi_{l-l'}(Q_l - Q_{l'})^2$$
$$+ W'(c) \sum_{l \in \Lambda} Q_l^2 + \frac{a}{2} \sum_{l \in \Lambda} Q_l^2 - h \sum_{l \in \Lambda} Q_l \tag{3.8}$$

and

$$c = \eta\left(\frac{1}{V} \sum_{l \in \Lambda} Q_l^2\right) = \eta(Q_0^2) \tag{3.9}$$

*Proof.* Comparing the original Hamiltonian (3.1) and the effective one (3.8), we may concentrate our attention on the $W$ term in the Hamiltonian. Consider then the function $W$ as given by its series expansion and treat it term by term. The proposition follows from the formula

$$\left[V\left(\frac{1}{V} \sum_{l \in \Lambda} Q_l^2\right)^n, A\right]$$
$$= \sum_{k=0}^{n-1} \left(\frac{1}{V} \sum_{l \in \Lambda} Q_l^2\right)^k \left[\sum_{l \in \Lambda} Q_l^2, A\right] \left(\frac{1}{V} \sum_{l \in \Lambda} Q_l^2\right)^{n-k-1}$$

for all $A \in \mathscr{A}$, and from the property (3.7). Indeed,

$$\eta\text{-weak-}\lim_{\Lambda} \left[V\left(\frac{1}{V} \sum_{l \in \Lambda} Q_l^2\right)^n, A\right]$$
$$= \sum_{k=0}^{n-1} \eta(Q_0^2)^k \left[\sum_l Q_l^2, A\right] \eta(Q_0^2)^{n-k-1}$$
$$= n\eta(Q_0^2)^{n-1} \left[\sum_l Q_l^2, A\right] \quad \blacksquare$$

By this proposition the derivation $\delta_h^\eta$ can be weakly approximated by the commutator with the effective Hamiltonian $H_\Lambda^\eta(h)$ of (3.8), which is at most quadratic in the observables $Q$ and $P$. Hence its equilibrium and ground states, solutions of (3.5) and (3.6), can be calculated explicitly. The ergodic equilibrium states $\eta$ are convex combinations of so-called quasifree of generalized free states (ref. 14, Sections 5.2 and 5.3) of the algebra of observables $\mathscr{A}$ generated by the canonical operators $Q_l$ and $P_{l'}$, $l, l' \in \mathbb{Z}^d$.

Generalized free states have the interesting property that they are completely characterized by the one- and two-point functions: $\eta(Q_l)$, $\eta(P_l)$, $\eta(Q_l Q_{l'})$, $\eta(P_l P_{l'})$, and $\eta(Q_l P_{l'})$, $l, l' \in \mathbb{Z}^d$.

In our model, because of time-reversal symmetry invariance, we have already $\eta(P_l) = 0$ and $\eta(Q_l P_{l'}) = 0$. Therefore, in order to characterize completely the solutions of (3.5) and (3.6), we have to compute only $\eta(Q_l)$, $\eta(Q_l Q_{l'})$, and $\eta(P_l P_{l'})$.

In fact, in order to characterize completely the state $\eta$, it remains to compute $\eta(Q_l)$.

If the external field $h = 0$, then the model $H^{\eta}_{\Lambda}(0)$ [as well as (3.1)] has the $\mathbb{Z}^2$ symmetry, i.e., the local Hamiltonians are invariant under the substitution $Q_l \to -Q_l$.

The model has been primarily invented to describe the phenomenon of the spontaneous breaking of this symmetry and the *softening* of the phonon mode $\Omega_{q=0}$; see (2.6). In the following we give a rigorous proof of this phenomenon. We follow the usual method, namely we consider the case $h \neq 0$ and discuss the limit $h \to 0$.

So let $h \neq 0$, and compute again, in terms of the dual lattice $\Lambda^*$, the self-consistency equation (3.9); the order parameter $c$ of (3.9) now depends on the external field and is denoted now by $c_h$ [cf. (2.10) and (A.15)]; then

$$c_h = \frac{h^2}{\Delta^2(c_h)} + \lim_{\Lambda} \frac{1}{V} \frac{\lambda}{[\Delta(c_h)]^{1/2}} \coth \frac{\beta\lambda}{2} [\Delta(c_h)]^{1/2} + I_d(c_h, T, \lambda) \tag{3.10}$$

where, as above, $\Delta(c) = a + 2W'(c)$; $c \in D$ [see (2.7)].

If $h \neq 0$, because $\Delta(c^*) = 0$, the $h^2$ term in (3.10) has a singularity at $c^*$ and Eq. (3.10) always has a solution $c_h > c^*$, i.e., $\Delta(c_h) > 0$; therefore, the second term in the right-hand side of (3.10) vanishes in the limit $\Lambda \to \infty$. We get $c_{h,\Lambda} \to c_h$ and the equation

$$c_h = \frac{h^2}{\Delta^2(c_h)} + I_d(c_h, T, \lambda) \tag{3.11}$$

Now we compute the expectation value of the average displacement operator

$$\eta(Q_0) = \lim_{\Lambda} \frac{1}{V} \eta\left(\sum_{l \in \Lambda} Q_l\right) = \frac{h}{\Delta(c_h)} \tag{3.12}$$

which is uniquely defined and different from zero, at least if $h \neq 0$. We have to consider two cases corresponding to the two phase regions (I) and (II) of Proposition 2.1 (see Fig. 1):

*Phase(I)*. In this case $c^* < I_d(c^*, T, \lambda)$ (see Fig. 2) and (3.11) has a solution $c_h$ such that

$$\lim_{h \to 0} c_h = c(T, \lambda) \geqslant c^*$$

Therefore, from (3.12)

$$\lim_{h \to 0} \eta(Q_0) = 0$$

*Phase (II)*. In this case $c^* > I_d(c^*, T, \lambda)$ (see Fig. 2). As in the proof of Proposition 2.1, using that $c \to c - I_d(c, T, \lambda)$ is monotonically increasing, (3.11) becomes in the limit $h \to 0$

$$\rho(T, \lambda) = c^* - I_d(c^*, T, \lambda) = \lim_{h \to 0} \frac{h^2}{\Delta(c_h)^2} > 0$$

Therefore, together with (3.12) one obtains

$$\eta_\pm(Q_0) = \lim_{h \to \pm 0} \eta(Q_0) = \pm[\rho(T, \lambda)]^{1/2} \tag{3.13}$$

or

$$\eta_+(Q_0) = -\eta_-(Q_0) = [\rho(T, \lambda)]^{1/2}$$

Clearly, this formulas hold in both regions now, but $\eta_\pm(Q_0) \neq 0$ in the phase region (II), i.e., in the limit $h \to 0$, there exist two different solutions $\eta_+$ and $\eta_-$ of both Eqs. (3.5) and (3.6) for $T < T_c(\lambda)$. Both solutions are not $Z^2$-symmetric, i.e., we have proved the spontaneous breaking of this symmetry. As expected, the average displacement value (3.13) is a nontrivial order parameter. Using the results of Proposition 2.1, one gets immediately the curves in Fig. 3 for the order parameter as a function of the temperature.

We collect all this in the following result.

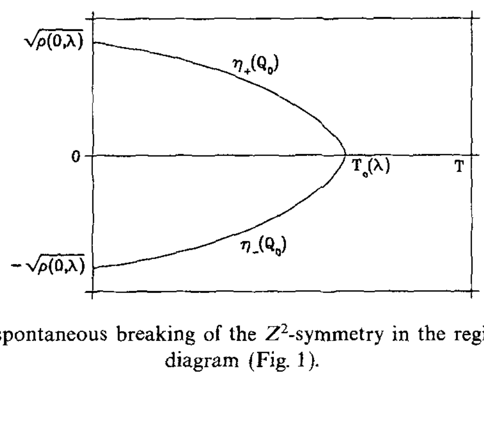


Fig. 3. Soft mode spontaneous breaking of the $Z^2$-symmetry in the region (II) of the phase diagram (Fig. 1).

**Proposition 3.2.** The model (2.1) shows a phase separation line $l_c(T)$ or $T_c(\lambda)$ (Proposition 2.1) showing spontaneous $Z^2$-symmetry breaking in the phase region (II). There exist two extremal equilibrium (or ground states) $\eta_+$ and $\eta_-$ on $\mathscr{A}$ such that

$$\eta_+(Q_0) = -\eta_-(Q_0) = [\rho(T, \lambda)]^{1/2} \neq 0, \qquad (T, \lambda) \in \text{(II)} \quad \blacksquare$$

## 4. FLUCTUATION OPERATORS

In this section our calculations are guided by the ideas recently developed in ref. 11, which create the possibility of making a clear distinction between classical fluctuations and fluctuations of a pure quantum nature. Although not explicitly stated, an embryonic form of these ideas is already inherent in the work of Hepp and Lieb[15] on laser theory.

The theory has already served[16] to give the microscopic explanation of the self-consistent phonon theory in solid state physics, yielding a full particle description of phonons.

Here we use from ref. 3 essentially two things: first, the notion of a fluctuation as an operator and second, the frame in which it is possible to give the joint description of two and more fluctuations, giving a meaning to the algebra of fluctuations.

Without going into the details, let us introduce the notions and the essentials of this theory.

Consider $A_i$ a copy of a local operator $A$ at the lattice site $i \in \mathbb{Z}^d$. In refs. 3 and 4 it is proved that one can give a meaning to these limits

$$F_0(A) = \lim_{\Lambda} \frac{1}{\sqrt{V}} \sum_{i \in \Lambda} [A_i - \eta(A)] \tag{4.1}$$

as unbounded operators on some Hilbert space, for every ergodic state $\eta$ on the algebra $\mathscr{A}$, which is enough clustering. The limit is in the sense of the usual central limit theorem in probability, but now with respect to the state $\eta$. The operator $F_0(A)$ is called, in a natural way, the *fluctuation operator* of $A$ in the state $\eta$. Technically, the existence of the fluctuation operator is guaranteed if one proves that the variance of the fluctuation is not trivial, in particular one has to prove

$$0 < \lim_{\Lambda} \eta\left(\left\{\frac{1}{\sqrt{V}} \sum_{i \in \Lambda} [A_i - \eta(A)]\right\}^2\right) < \infty \tag{4.2}$$

Consider now the following commutator: take two local operators $A, B \in \mathscr{A}$,

$$\left[\frac{1}{\sqrt{V}} \sum_{i \in \Lambda} [A_i - \eta(A)], \frac{1}{\sqrt{V}} \sum_{j \in \Lambda} [B_j - \eta(B)]d = \frac{1}{V} \sum_{i \in \Lambda} [A_i, B_i] \right. \tag{4.3}$$

where we used the local commutativity

$$[A_i, B_j] = \delta_{ij}[A_i, B_i]$$

Take the weak-limit $\Lambda \to \mathbb{Z}^d$ of (4.3) in the state $\eta$; then one gets

$$\begin{aligned}[F_0(A), F_0(B)] &= \lim_{\Lambda} \frac{1}{V} \sum_{i \in \Lambda} [A_i, B_i] \\ &= \eta([A, B]) \end{aligned} \tag{4.4}$$

The second equality is due to the ergodicity of the state $\eta$.

Equation (4.4) is a nontrivial canonical commutation relation between the fluctuation operators $F_0(A)$ and $F_0(B)$ if the $c$-number $\eta([A, B]) \neq 0$. It indicates the *quantum character* of the fluctuations. In fact ref. 3 proves that $F_0(A)$ and $F_0(B)$ are boson fields.

The *normality* of the fluctuation defined by (4.1) is manifested by the factor $1/\sqrt{V}$ in front of the sum.

In this paper we generalize the central limit result (4.1) in two directions:

(a) We consider fluctuation operators $F_\delta(A)$ of the type (4.1), but which carry a normalization factor $V^{-1/2-\delta}$ with $\delta \in (-1/2, 1/2)$; the *critical exponent* $\delta$ measures the deviation from the standard square root; it measures the degree of criticality of the corresponding fluctuation operator. Comparing with (4.2), we have now to check the $\delta \in (-1/2, 1/2)$ for which the following variance is nontrivial:

$$0 < \lim_{\Lambda} \eta \left( \left\{ \frac{1}{V^{1/2+\delta}} \sum_{i \in \Lambda} [A_i - \eta(A)] \right\}^2 \right) < \infty \tag{4.5}$$

Following the general results of refs. 3 and 4, if (4.5) holds, it defines the fluctuation operator

$$F_\delta(A) = \lim_{\Lambda} \frac{1}{V^{1/2+\delta}} \sum_{i \in \Lambda} [A_i - \eta(A)] \tag{4.6}$$

If $\delta > 0$, then $F_\delta(A)$ is called an *abnormal critical* fluctuation; if $\delta < 0$ it is called a *supernormal (sqeezed) critical* fluctuation.

Again one can consider the commutator of two fluctuation operators [compare with (4.3) and (4.4)]

$$[F_\delta(A), F_{\delta'}(B)] = \lim_{\Lambda} \frac{1}{V^{1+\delta+\delta'}} \sum_{i \in \Lambda} [A_i, B_i]$$

$$= \begin{cases} \eta([A, B]) & \text{if} \quad \delta + \delta' = 0 \\ 0 & \text{if} \quad \delta + \delta' > 0 \\ \text{undefined} & \text{if} \quad \delta + \delta' < 0 \end{cases} \tag{4.7}$$

This is again a way for distinguishing between the classical and quantum character of the fluctuations.

(b) Motivated by the work of Ellis and Newman,[6] we also consider fluctuation operators $F_\delta(A)$ of the type (4.6), but where the central limit is taken in a very specific way. One takes simultaneously the limit for the size of the system together with the number of random variables. To be precise, let $\{\eta_\Lambda\}_\Lambda$ be a sequence of finite-volume Gibbs states, such that $\lim_\Lambda \eta_\Lambda = \eta$ is an *ergodic* limit state, then check the $\delta \in (-1/2, 1/2)$ for which the following variance is nontrivial:

$$0 < \lim_\Lambda \eta_\Lambda \left( \left\{ \frac{1}{V^{1/2+\delta}} \sum_{i \in \Lambda} [A_i - \eta_\Lambda(A)] \right\}^2 \right) < \infty \tag{4.8}$$

Again following the general theory,[3,4] this yields the fluctuation operator

$$F_\delta(A) = \lim_\Lambda \frac{1}{V^{1/2+\delta}} \sum_{i \in \Lambda} [A_i - \eta_\Lambda(A)] \tag{4.9}$$

Remark that defining the limits in the sense of (4.5) or of (4.8) does not make any difference in the search for the classical or quantum nature of the fluctuations, because in the commutator the scalar term drops out immediately.

In our model we consider the fundamental observables of momentum and displacement, in particular

$$F_\delta(Q) = \lim_\Lambda \frac{1}{V^{1/2+\delta}} \sum_{l \in \Lambda} [Q_l - \eta_\Lambda(Q_l)] \tag{4.10}$$

$$F_{\delta'}(P) = \lim_\Lambda \frac{1}{V^{1/2+\delta'}} \sum_{l \in \Lambda} [P_l - \eta_\Lambda(P_l)] \tag{4.11}$$

We have to find $\delta$ and $\delta'$ such that the variances in the sense of (4.8) are nontrivial. We take for $\{\eta_\Lambda\}_\Lambda$ any sequence of the Gibbs states determined by the effective Hamiltonian (3.8) with

$$c_\Lambda = \eta_\Lambda \left( \frac{1}{V} \sum_{l \in \Lambda} Q_l^2 \right)$$

[compare to (3.9)], and such that the $\eta_\Lambda$ tend to the unique solution $\eta$ for $(T, \lambda)$ in the phase region (I); for $(T, \lambda)$ in the phase region (II), the $\eta_\Lambda$ tend to the extremal states $\eta_+$ or $\eta_-$; see Proposition 3.3. Then we have the following result.

**Proposition 4.1**. If $(T, \lambda)$ belongs to the region (I), then $\delta=\delta'=0$, i.e., the fluctuation operators $F_0(Q)$ and $F_0(P)$ are normal. Furthermore,

$$[F_0(P), F_0(Q)] = \frac{\hbar}{i}$$

The Algebra of fluctuations is of quantum nature.

*Proof*. Straightforward computation yields

$$\eta_A\left(\left\{\frac{1}{V^{1/2+\delta}} \sum_{l \in A} [Q_l - \eta_A(Q_l)]\right\}^2\right) = \frac{1}{V^{2\delta}} \frac{\lambda}{[\Delta(c_A)]^{1/2}} \coth\frac{\beta\lambda}{2} [\Delta(c_A)]^{1/2} \tag{4.12}$$

and

$$\eta_A\left(\left(\frac{1}{V^{1/2+\delta'}} \sum_{l \in A} P_l\right)^2\right) = \frac{1}{V^{2\delta'}} \frac{\lambda m}{2} [\Delta(c_A)]^{1/2} \coth\frac{\beta\lambda}{2} [\Delta(c_A)]^{1/2} \tag{4.13}$$

From Section 3, proof of Proposition 3.1, we get that $\lim_A c_A = c > c^*$; hence there is a finite gap $\Delta(c) > 0$; therefore, the limits $A \to \infty$ of (4.12) and (4.13) are nontrivial if and only if $\delta=\delta'=0$. The commutation relation is as in (4.4) or (4.7). ∎

**Proposition 4.2.** If $0 < T < T_c(\lambda)$ [region (II)], then the momentum fluctuation operator $F_0(P)$ is normal; the displacement fluctuation operator is of the type $F_\delta(Q)$ with $0 < \delta \leqslant 1/2$, where $\delta$ depends on the boundary condition (see below). The fluctuation algebra is Abelian.

*Proof*. As indicated in Proposition 3.3, we take first $A \to \mathbb{Z}^d$ and then $h \to 0$. If $h \to 0$, then the solution $c(h)$ of the self-consistency equation (2.11) tends to $c^*$ and $\Delta(c_h) \to \Delta(c^*) = 0$.

The normality of the momentum fluctuation operator follows immediately from the expression (4.13), i.e., $\delta'=0$. The displacement operator is somewhat more delicate. We start from the situation $h \neq 0$. Consider the formula (3.12):

$$\eta(Q_0) = \frac{h}{\Delta(c_h)}$$

i.e., both fluctuation operators are normal ($\delta=\delta'=0$) for $h \neq 0$. From (3.13), $\Delta(c_h) \simeq |h| [\rho(T, \lambda)]^{1/2}$ for small $h$. Clearly, from (4.12) we do not have any nontrivial variance for $Q$ in the limit $h \to 0$ (*after* $A \to \mathbb{Z}^d$ for $\delta=0$). We have to take special boundary conditions.[17,18] We take

$$h = \frac{\hat{h}}{V^\alpha} \tag{4.14}$$

with $\hat{h}$ fixed and $\alpha > 0$, i.e., we couple $\lim h \to 0$ to $\lim \Lambda \to \mathbb{Z}^d$. We consider three regimes:

(a) $0 < \alpha < 1$. Considering the self-consistency equation (3.10) and $\lim \Lambda \to \mathbb{Z}^d$, we see that the zero-mode term does not contribute and we obtain

$$0 < \rho(T, \lambda) = \lim_{\Lambda \to \mathbb{Z}^d} \left( \frac{\hat{h}}{V^\alpha \Delta(c_{h,\Lambda})} \right)^2 = c^* - I_d(c^*, T, \lambda) < \infty$$

Hence

$$\lim_\Lambda \eta(Q_0) = \lim_\Lambda \frac{\hat{h}}{V^\alpha \Delta(c_{h,\Lambda})} = (\text{sign}\, \hat{h})[\rho(T, \lambda)]^{1/2}$$

Therefore formula (4.12) becomes

$$0 < \lim_\Lambda \eta_\Lambda \left( \left\{ \frac{1}{V^{1/2+\delta}} \sum_{l \in \Lambda} [Q_l - \eta_\Lambda(Q_l)] \right\}^2 \right) = \lim_\Lambda \frac{1}{V^{2\delta-\alpha}} \frac{[\rho(T, \lambda)]^{1/2}}{\beta |\hat{h}|} < \infty \tag{4.15}$$

implying $2\delta = \alpha$ or $0 < \delta < 1/2$, depending on the boundary condition (4.14).

(b) $\alpha = 1$. Then in formula (3.10), the $h$ term as well as the zero-mode term contribute and one gets

$$\begin{aligned} 0 < \rho(T, \lambda) &= \lim_\Lambda \left\{ \frac{\hat{h}^2}{(\Delta(c_{h,\Lambda}) V)^2} + \frac{1}{\beta(\Delta(c_{h,\Lambda}) V)} \right\} \\ &= c^* - I_d(c^*, T, \lambda) < \infty \end{aligned}$$

Therefore

$$0 < x \equiv \lim_\Lambda \Delta(c_{h,\Lambda}) V < \infty$$

Hence

$$\rho(T, \lambda) = \frac{\hat{h}^2}{x^2} + \frac{1}{\beta x}$$

and

$$\lim_\Lambda \eta(Q_0) = \lim_\Lambda \frac{\hat{h}}{\Delta(c_{h,\Lambda}) V} = \frac{\hat{h}}{x} < [\rho(T, \lambda)]^{1/2}$$

or

$$\eta_-(Q_0) < \lim_\Lambda \eta(Q_0) < \eta_+(Q_0)$$

i.e., $\eta$ is a convex combination of $\eta_+$ and $\eta_-$:

$$\eta = \lambda\eta_+ + (1-\lambda)\eta_- \tag{4.16}$$

and for $\rho = \rho(T, \lambda)$ one gets

$$\frac{\hat{h}}{x} = \lambda\sqrt{\rho} - (1-\lambda)\sqrt{\rho}$$

or

$$\lambda = \frac{1}{2}\left(1 + \frac{\hat{h}}{x\sqrt{\rho}}\right)$$

Furthermore, $x$ can also be computed from the equation for $\rho = \rho(T, \lambda)$:

$$x = \frac{1}{2\beta\rho} + \left(\frac{1}{4\beta^2\rho^2} + \frac{\hat{h}^2}{\rho}\right)^{1/2} > 0$$

Remark that the standard quasiaverage approach, $h \to \pm 0$ *after* $\Lambda \to \mathbb{Z}^d$ (see, e.g., refs. 17 and 18), corresponds to $\hat{h} \to \pm\infty$ in (4.16). In any event, the computation of fluctuations in a *mixed state* is not so relevant. By (4.15) it yields always $\delta = 1/2$, i.e., *abnormal fluctuations* corresponding to the mixed phases.

(c) $\alpha > 1$. Considering again (3.10), the external field term is small with respect to the zero-mode term and one has

$$0 < \rho(T, \lambda) = \lim_\Lambda \frac{1}{\beta\Delta(c_{h,\Lambda})V} = c^* - I_d(c^*, T, \lambda) < \infty$$

Hence for large $\Lambda$, $\Delta(c_h) \simeq V^{-1}$, yielding

$$\lim_\Lambda \eta(Q_0) = \lim_\Lambda \frac{\hat{h}}{\Delta(c_{h,\Lambda})V^\alpha} = 0$$

and $\delta = 1/2$ [see (4.12)] together with

$$\eta = \tfrac{1}{2}\eta_+ + \tfrac{1}{2}\eta_-$$

Formally this result corresponds to $\hat{h} \downarrow 0$ in (4.16). Again the limit state is not extremal. Finally, as far as the boundary condition (4.14) is concerned, only the case (a), $0<\alpha<1$, yields an *extremal state* with fluctuation operators as indicated in the proposition, i.e., $\delta=\alpha/2$, $\delta'=0$. Following (4.7), the fluctuation algebra is Abelian. ∎

Remark that we have considered a very special boundary condition (4.14); one can of course argue using other types of boundary conditions. Here we only wanted to stress the sensitivity of the fluctuations to the boundary conditions.

Now we proceed with our results for $(T, \lambda)$ on the critical line, i.e., $(T, \lambda)$ satisfies the equation $c^*=I_d(c^*, T, \lambda)$.

**Proposition 4.3.** If $(T, \lambda)$ belongs to the critical line $(T, \lambda_c(T))$ or $(T_c(\lambda), \lambda)$ (see Fig. 1), but $T>0$ or $T_c(\lambda)>0$, then the momentum fluctuation operator $F_0(P)$ is normal, the displacement fluctuation operator $F_\delta(Q)$ is abnormal critical with a critical exponent $\delta$ which is dimension dependent:

$$\delta_d=\begin{cases}\frac{1}{3} & \text{if } f=3\\ \frac{1}{4}+0 & \text{if } d=4\\ \frac{1}{4} & \text{if } d\geqslant 5\end{cases}$$

The algebra of fluctuation operators is Abelian.

*Proof.* We must carefully study how the self-consistency equation (3.10) tends to the critical line $c^*=I_d(c^*, T_c(\lambda), \lambda)$ if $T_c(\lambda)>0$. From this we must find out how the energy gap $\Delta(c_\Lambda)$ behaves as a function of the volume. Clearly, if $\Lambda$ tends to infinity,

$$\lim_\Lambda \frac{1}{V}\frac{\lambda}{2[\Delta(c_\Lambda)]^{1/2}}\coth\frac{\beta_c(\lambda)\lambda}{2}[\Delta(c_\Lambda)]^{1/2}=0$$

or

$$\lim_\Lambda \frac{1}{V\Delta(c_\Lambda)}=0$$

We choose a behavior $\Delta(c_\Lambda)\simeq O(V^{-\gamma})$ with $\gamma<1$ and try to find explicitly this parameter $\gamma$.

Write formula (3.10) in the form

$$\begin{aligned}c_\Lambda-c^*+\{c^*-I_d(c_\Lambda, T_c(\lambda), \lambda)\}\\ +\left\{I_d(c_\Lambda, T_c(\lambda), \lambda)-\frac{1}{V}\sum_{q\neq 0}\frac{\lambda}{2\Omega_q}\coth\frac{\beta_c(\lambda)\lambda}{2}\Omega_q(c_\Lambda)\right\}\\ =\frac{1}{V}\frac{\lambda}{2[\Delta(c_\Lambda)]^{1/2}}\coth\frac{\beta_c(\lambda)\lambda}{2}[\Delta(c_\Lambda)]^{1/2}\end{aligned} \tag{4.17}$$

where $I_d$ is the integral (2.12). First we look at the second term in curly brackets in formula (4.17). Using

$$\tilde{\phi}(0)-\tilde{\phi}(q)=s^2q^2+O(q^2); \qquad s>0$$

for small $q$ and

$$\frac{\lambda}{2\Omega_q}\coth\frac{\beta\lambda}{2}\Omega_q\leqslant\frac{1}{\beta\Omega_q^2}\leqslant\frac{1}{\beta s^2q^2}$$

yields directly, using formula (A.7) of ref. 19,

$$I_d(c_\Lambda, T_c, \lambda_c)-\frac{1}{V}\sum_{q\neq 0}\frac{\lambda_c}{2\Omega_q}\coth\frac{\beta_c\lambda_c}{2}\Omega_q=O(V^{-(d-\sigma)/d})|_{\sigma=2} \tag{4.18}$$

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

$$I_d(c, T, \lambda)=\frac{1}{(2\pi)^d}\int_{\mathfrak{B}_d} d^dk\,\frac{\lambda}{2\Omega_q}\coth\frac{\beta\lambda}{2}\Omega_q$$

Therefore

$$\begin{aligned}
c^*-I_d(c_\Lambda)&=I_d(c^*)-I_d(c_\Lambda)\\
&=I_d^{(<\varepsilon)}(c^*)-I_d^{(<\varepsilon)}(c_\Lambda)+I_d^{(>\varepsilon)}(c^*)-I_d^{(>\varepsilon)}(c_\Lambda)\\
&=\frac{\Delta(c_\Lambda)}{\beta_c(2\pi)^d}\int_{|q|<\varepsilon} d^dq\,\frac{1}{s^2q^2(\Delta(c_\Lambda)+s^2q^2)}\\
&\quad+(c_\Lambda-c^*)\,\partial_c I_d^{(>\varepsilon)}(c'_\Lambda)
\end{aligned}$$

Remark also that $\Delta(c_\Lambda)=(c_\Lambda-c^*)\,2W''(c^*)+o(c_\Lambda-c^*)$, or

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

Hence

$$\begin{aligned}
&c^*-I_d(c_\Lambda, T_c(\lambda), \lambda)\\
&\quad=\frac{\Delta(c_\Lambda)}{\beta_c(\lambda)(2\pi)^d}\int_{|q|<\varepsilon} d^dq\,\frac{1}{s^2q^2(\Delta(c_\Lambda)+s^2q^2)}\\
&\qquad+\frac{\Delta(c_\Lambda)}{2W''(c^*)}\,\partial_c I_d^{(>\varepsilon)}(c'_\Lambda)+O(c_\Lambda-c^*)
\end{aligned}$$

A straightforward computation yields

$$I_3^{(<\varepsilon)}(c^*) - I_3^{(<\varepsilon)}(c_A) = \frac{4\pi}{\beta_c(\lambda)(2\pi)^3 s^3} [\Delta(c_A)]^{1/2} \operatorname{arctg} \frac{s\varepsilon}{[\Delta(c_A)]^{1/2}}$$

$$I_4^{(<\varepsilon)}(c^*) - I_4^{(<\varepsilon)}(c_A) = \frac{K}{\beta_c(\lambda) s^4} \Delta(c_A) \ln \frac{s^2\varepsilon^2 + \Delta(cA)}{\Delta(c_A)}$$

where $K$ is a constant; for $d \geqslant 5$ we can work with the formula

$$I_d(c^*) - I_d(c_A) = (c_A - c^*)\, \partial_c I_d(c'_A)$$

Now we are in a position to rewrite Eq. (4.17), using all these results. If $d=3$, then (4.17) becomes, in the limit $\Lambda \to \mathbb{Z}^3$, as $\Delta(c_A) \to 0$,

$$\left\{ \frac{\Delta(c_A)}{2W''(c^*)} + \frac{4\pi}{\beta_c(\lambda)(2\pi)^3 s^3} [\Delta(c_A)]^{1/2} \operatorname{arctg} \frac{s\varepsilon}{[\Delta(c_A)]^{1/2}} \right.$$
$$\left. + \frac{\Delta(c_A)}{2W''(c^*)} \partial_c I_d^{(>\varepsilon)}(c'_A) + O(V^{-(3-2)/3}) \right\} V\beta_c(\lambda)\Delta(c_A) = 1$$

The only solution of this equation is

$$\Delta(c_A) \simeq V^{-2/3} \tag{4.19}$$

and only the second and the fourth terms within the brackets contribute. If $d=4$, then (4.17) becomes

$$\left\{ \frac{\Delta(c_A)}{2W''(c^*)} + \frac{K}{\beta_c(\lambda) s^4} \Delta(c_A) \ln \frac{s^2\varepsilon^2 + \Delta(c_A)}{\Delta(c_A)} \right.$$
$$\left. + \frac{\Delta(c_A}{2W''(c^*)} \partial_c I_d^{(>\varepsilon)}(c'_A) + O(V^{-(4-2)/4}) \right\} V\beta_c(\lambda)\, \Delta(c_A) = 1$$

The only solution for $\Delta(c_A)$ is

$$\Delta(c_A) \simeq \frac{1}{V^{1/2} \ln V} \tag{4.20}$$

again this behavior is determined by the second and the fourth terms. If $d=5$, then

$$\left\{ \frac{\Delta(c_A)}{2W''(c^*)} + \frac{\Delta(c_A)\, \partial_c I_d(c'_A)}{2W''(c^*)} + O(V^{-(5-2)/5}) \right\} V\beta_c(\lambda)\, \Delta(c_A) = 1$$

The only solution is

$$\Delta(c_A) \simeq V^{-1/2} \tag{4.21}$$

This behavior is determined by the first and second terms in the brackets, and clearly this result holds also for all dimensions $d \geqslant 5$.

Now we turn to the computation of the fluctuations. We have to search for the value $\delta$ in order that the conditions (4.8) are satisfied. Using again formula (4.12), we get for the displacement variable at the critical line with $T_c(\lambda) > 0$

$$0 < \lim_{\Lambda} \eta_\Lambda \left( \left\{ \frac{1}{V^{1/2+\delta}} \sum_{l \in \Lambda} [Q_l - \eta_\Lambda(Q_l)] \right\}^2 \right) = \lim_{\Lambda} \frac{1}{V^{2\delta}} \frac{T_c(\lambda)}{\Delta(c_\Lambda)} < \infty$$

Using (4.19)–(4.21), one finds immediately that $\delta$ is dimension dependent and given by

$$\delta_d = \begin{cases} \frac{1}{3} & \text{for} \quad d = 3 \\ \frac{1}{4} + 0 & \text{for} \quad d = 4 \\ \frac{1}{4} & \text{for} \quad d \geqslant 5 \end{cases}$$

For the momentum fluctuation, from (4.13) one gets immediately that the critical exponent $\delta' = 0$ independent of the dimension.

That the algebra of fluctuation operators is Abelian follows from these results and from formula (4.7).

This proves the proposition. ∎

The Abelian or classical character of the fluctuation operators at criticality proved in the previous proposition is a rigorous result in complete correspondence with the standard wisdom that the quantum nature of the phase transition is suppressed at criticality. Finally, there is one more point to study in the phase diagram. This gives the following result.

**Proposition 4.4.** If $(T, \lambda)$ is the point $[T_c(\lambda) = 0, \lambda_c(0)]$, (i.e., at the pure quantum transition; see Fig. 1), then the displacement fluctuation operator $F_\delta(Q)$ is abnormal critical with a dimension-dependent critical exponent:

$$\delta_d = \begin{cases} \frac{1}{4} & \text{for} \quad d = 2 \\ \frac{1}{6} + 0 & \text{for} \quad d = 3 \\ \frac{1}{6} & \text{for} \quad d \geqslant 4 \end{cases}$$

Furthermore, the momentum fluctuation operator $F_{\delta'}(P)$ is supernormal (squeezed) critical with critical exponent $\delta' = -\delta_d$, where $\delta_d$ is an above.

It follows immediately that the algebra of fluctuation operators is non-Abelian, reflecting the quantum character of the phase transition; in particular,

$$[F_{\delta_d}(Q), F_{-\delta_d}(P)] = i\hbar\mathbb{1}$$

*Proof.* Here again we are at criticality and the gap $\Delta(c_\Lambda) \to 0$ if $\Lambda \to \mathbb{Z}^d$. We proceed in exactly the same way as in the proof of Proposition 4.3. However, the Equation (3.10) reads

$$c_\Lambda = \frac{\lambda}{2V[\Delta(c_\Lambda)]^{1/2}} + \frac{1}{V}\sum_{q\neq 0} \frac{\lambda}{2\Omega_q(c_\Lambda)}$$

with $\Omega_q(c) \simeq [\Delta(c) + s^2q^2]^{1/2}$ for small $q$. Recall also that

$$I_d(c^*, 0, \lambda_c) < \infty \qquad \text{for all} \quad d > 1$$

Again we use the approximation of the integral $I_d$ by sums over the duals of the finite volumes, i.e., we use again formula (A.7) of ref. 19; in this case $\sigma = 1$ [cf. (4.18)]. The explicit calculation of the integral around the singular point $q = 0$ yields now

$$\Delta(c_\Lambda) = \begin{cases} V^{-1} & \text{if} \quad d = 2 \\ (V^{2/3} \ln V)^{-1} & \text{if} \quad d = 3 \\ V^{-2/3} & \text{if} \quad d \geq 4 \end{cases}$$

Using these results and (4.12), one gets a solution $\delta$ for (4.12) and $\beta = \infty$:

$$0 < \tilde{\eta}(F_\delta(Q)^2) = \lim_\Lambda \frac{1}{V^{2\delta}} \frac{\lambda_c(0)}{[\Delta(c_\Lambda)]^{1/2}} < \infty$$

given by

$$\delta = \delta_d = \begin{cases} \frac{1}{4} & \text{if} \quad d = 2 \\ \frac{1}{5} + 0 & \text{if} \quad d = 3 \\ \frac{1}{6} & \text{if} \quad d \geq 4 \end{cases}$$

The computation of $\delta'$ is now also immediate from the formula (4.13) for $\beta = \infty$:

$$0 < \eta(F_{\delta'}(P)^2) = \lim_\Lambda \frac{1}{V^{2\delta'}} \frac{\lambda_c(0)m}{2} [\Delta(c_\Lambda)]^{1/2} < \infty$$

i.e., $\delta' = -\delta_d$.

Finally, the nontriviality of the commutation relation is immediate from (4.7). ∎

## 5. CONCLUDING REMARKS

We found a structural phase transition at $\lambda_c(0)$, $T_c = 0$, where the algebra of fluctuation operators is non-Abelian and the critical exponents $\delta$, $\delta' \neq 0$. This is a manifestation of the pure quantum nature of the phase transition. In contrast to the so-called temperature transitions [$T_c(\lambda) > 0$, Proposition 4.3], we get here a rigorous analysis of a phase transition where one detects quantum features at criticality at the macroscopic level of its fluctuations. The very specific property is that the degree of abnormality in the fluctuations of the displacement is counterbalance by the same degree of supernormal criticality or the squeezing of the momentum fluctuation.

It would be instructive even from an experimental point of view to proceed with the further study of this phenomenon in quantum many-body systems of solid state physics. The effect of squeezing is well known and intensively studied in quantum optics (see, e.g., ref. 20). Which are the devices to measure it in solid state physics and what are the possible applications?

As far as our model is concerned, the phenomenon is present only at $T = 0$. This comes as an artifact of the model. In real physics this phenomenon should be observed in a "neighborhood" of $T = 0$.

Another way of looking at the phenomenon is to consider it as an expression of an uncertainty principle for criticality in quantum systems.

Finally, compared the degree of criticality in the case of temperature-driven transitions, i.e., $\delta_d$ in Proposition 4.3, with the degree of the pure quantum transition, i.e., $\delta_d$ in Proposition 4.4. One remarks that the quantum fluctuations are less critical than the corresponding classical ones. Intuitively this is obviously a consequence of the quantum tunneling effects which become manifest at $T = 0$.

Before finishing, we mention that we did not discuss here the problem of the dynamics of the fluctuations, which is classified in ref. 3 within the general theory of normal fluctuations. The interesting aspect of our results here is situated within the critical fluctuations. An extension of the existing theory to our situation should be elaborated first. We leave it to a future contribution. On that occasion we hope to be able to clarify the connection of the fluctuation spectrum with the soft-mode spectrum for the displacement structural phase transition. We hope to be able to clarify the so-called central peak problem which is believed to be connected with the intimate relation of the central mode with the critical fluctuations near a structural phase transition.

An extension of our results to the case of more degrees of freedom per lattice site is also under current research. The symmetry breaking is more complicated and new types of fluctuations are in order.

## APPENDIX. CALCULATION OF THE FREE ENERGY DENSITY

To calculate the thermodynamic limit of the free energy density $f_V[H_\Lambda(h)] = (-\beta V)^{-1} \ln \operatorname{Tr}(-\beta H_\Lambda(h))$, where [cf. (1.1) and (3.1)]

$$H_\Lambda(h) = T_\Lambda + VW\left(\frac{1}{V}\sum_{l\in\Lambda} Q_l^2\right) - h\sum_{l\in\Lambda} Q_l \tag{A.1}$$

we suppose that the real function $W\colon \mathbb{R}^1_+ \to \mathbb{R}^1$ satisfies the following conditions:

$$\begin{aligned} &\text{(i)} \quad W(x) \geqslant B \quad (\text{or} \quad > -\tfrac{1}{2}ax) \\ &\text{(ii)} \quad 0 < \partial_x^2 W(x) \leqslant \varepsilon \end{aligned} \tag{A.2}$$

**Lemma A1.** Let the self-adjoint operator $T_{\Lambda,a}$ in the Hilbert space $\mathscr{H}_\Lambda = \otimes_{l\in\Lambda} L^2(\mathbb{R}^1)$ be the generator of the Gibbs semigroup, i.e., for $\beta > 0$, $\exp(-\beta T_{\Lambda,a}) \in \text{Tr-class}(\mathscr{H}_\Lambda)$. Then $\exp(-\beta H_\Lambda(h)) \in \text{Tr-class}(\mathscr{H}_\Lambda)$ for any $h \in \mathbb{R}^1$.

*Proof.* Recall that the self-adjoint operator $T_{\Lambda,a}$ has the form [see (1.1)]

$$T_{\Lambda,a} = \sum_{l\in\Lambda} \frac{1}{2m} P_l^2 + \frac{1}{4}\sum_{l,l'\in\Lambda} \phi_{ll'}(Q_l - Q_{l'})^2 + \frac{a}{2} Q_l^2, \qquad a > 0 \tag{A.3}$$

Then, by condition (i), for any $h \in \mathbb{R}$, the operator

$$U_a(h) = \frac{a}{2}\sum_{l\in\Lambda} Q_l^2 + VW\left(\frac{1}{V}\sum_{l\in\Lambda} Q_l^2\right) - h\sum_{l\in\Lambda} Q_l \geqslant B(h)\cdot\mathbb{1} \tag{A.4}$$

is semibounded from below by a $B(h)$. Hence, the operator (A.1) is self-adjoint on the domain $D(T_{\Lambda,a})$. On this domain we can represent the operator (A.1) as a well-defined algebraic sum

$$H_\Lambda(h) = T_{\Lambda,a-\delta} + U_\delta(h), \qquad \delta > 0 \tag{A.5}$$

where $a - \delta > 0$, the first term corresponds to the operator (A.3) with parameter substituted by $a - \delta$, and the second term corresponds to the operator (A.4) with parameter $\delta > 0$. Then $U_\delta(h) \geqslant B(h)$ is semibounded from below, but $T_{\Lambda,a-\delta}$ is still a generator of the Gibbs semigroup. Hence, by the *Golden–Thompson inequality*

$$\operatorname{Tr}_{\mathscr{H}_\Lambda}(e^{-\beta H_\Lambda(h)}) \leqslant \operatorname{Tr}_{\mathscr{H}_\Lambda}(e^{-\beta T_{\Lambda,a-\delta}} e^{-\beta U_\delta(h)}) \tag{A.6}$$

one gets the statement of the lemma. ∎

Now we can construct an *approximating Hamiltonian* $H_\Lambda(c, h)$ using the following operator expansion:

$$H_\Lambda(h) = T_\Lambda - h \sum_{l\in\Lambda} Q_l + V\left\{W(c) + \left(\frac{1}{V}\sum_{l\in\Lambda} Q_l^2 - c\right) W'(c) + \frac{1}{2}\int_{\mathbb{R}^1_+} d\mathbb{E}_\lambda\left(\frac{1}{V}\sum_{l\in\Lambda} Q_l^2\right)(\lambda - c)^2 W''(c_\lambda)\right\} \tag{A.7}$$

Hence, in the last term, we use the spectral decomposition for the self-adjoint operator $(1/V)\sum_{l\in\Lambda} Q_l^2$ and the second derivative of the function $W(c)$ in the inermediate point $c_\lambda$. The part *linear* in the operator $(1/V)\sum_{l\in\Lambda} Q_l^2$ of the expansion (A.7) is called the *approximating* (or *trial*) Hamiltonian for the original one (A.1):

$$H_\Lambda(c, h) = T_\Lambda - h\sum_{l\in\Lambda} Q_l + W'(c)\sum_{l\in\Lambda} Q_l^2 + V\{W(c) - cW'(c)\} \tag{A.8}$$

**Theorem A1.** Let the function $W(x)$ describing the anharmonicity in the Hamiltonian (A.1) satisfy the conditions (A.2). Then the thermodynamic limit for the free energy density $\{f_V[\mathscr{H}_\Lambda(h)]\}_V$ exists and

$$\lim_V f_V[H_\Lambda(h)] = \lim_V \sup_c f_V[H_\Lambda(c, h)] \equiv f(T, h) \tag{A.9}$$

*Proof.* By the *Bogoliubov inequality* one gets

$$\frac{1}{V}\langle H_\Lambda(h) - H_\Lambda(c, h)\rangle_{H_\Lambda(h)} \leqslant f_V[H_\Lambda(h)] - f_V[H_\Lambda(c, h)] \leqslant \frac{1}{V}\langle H_\Lambda(h) - H_\Lambda(c, h)\rangle_{H_\Lambda(c,h)} \tag{A.10}$$

Here $\langle - \rangle_{H_\Lambda(h)}$ and $\langle - \rangle_{H_\Lambda(c,h)}$ are finite-volume Gibbs states defined by the full and approximating Hamiltonians, respectively. By the condition (ii) of (A.2) and by (A.7) and (A.8) we obtain

$$0 \leqslant \frac{1}{V}\langle H_\Lambda(h) - H_\Lambda(c, h)\rangle_{H_\Lambda(h)},$$

$$\frac{1}{V}\langle H_\Lambda(h) - H_\Lambda(c, h)\rangle_{H_\Lambda(c,h)} \leqslant \frac{1}{2}\varepsilon\left\langle\left(\frac{1}{V}\sum_{l\in\Lambda} Q_l^2 - c\right)^2\right\rangle_{H_\Lambda(c,h)}$$

Therefore, the inequality (A.10) gives the following estimate for the free energy density:

$$0 \leqslant f_V[H_\Lambda(h)] - \sup_c f_V[H_\Lambda(c, h)] \leqslant \frac{1}{2}\varepsilon\left\langle\left[\frac{1}{V}\sum_{l\in\Lambda} Q_l^2 - c_\Lambda(T, h)\right]^2\right\rangle_{H_\Lambda(c_\Lambda, h)} \tag{A.11}$$

where $c_\Lambda(T, h)$ corresponds to the point where the $\sup_c f_V[H(c, h)]$ is attained. Note that the approximating Hamiltonian (A.8) is a "renormalized" harmonic Hamiltonian with the frequencies

$$\Omega_k(c) = \{\Delta(c) + [\tilde{\phi}(0) - \tilde{\phi}(k)]\}^{1/2}, \qquad k \in \Lambda^* \tag{A.12}$$

where

$$\Delta(c) = a + 2W'(c) \tag{A.13}$$

Then by explicit calculations one gets

$$f_V[H_\Lambda(c, h)] = \frac{1}{\beta V} \sum_{k \in \Lambda^*} \ln\left[2 \operatorname{sh} \frac{1}{2} \beta\lambda\Omega_k(c)\right] - \frac{1}{2} \frac{h^2}{\Delta(c)} + [W(c) - cW'(c)] \tag{A.14}$$

and, correspondingly, the following equation for the point $c_\Lambda(T, h)$:

$$c_\Lambda(T, h) = \left\langle \frac{1}{V} \sum_{l \in \Lambda} Q_l^2 \right\rangle_{H_\Lambda(c_\Lambda, h)} = \frac{h^2}{\Delta^2(c_\Lambda)} + \frac{1}{V} \sum_{k \in \Lambda^*} \frac{\lambda}{2\Omega_k(c_\Lambda)} \coth \frac{1}{2} \beta\lambda\Omega_k(c_\Lambda) \tag{A.15}$$

where $\lambda = \hbar/\sqrt{m}$. In (A.15) we used condition (ii) of (A.2). Calculation of the expectation in the rhs of (A.11) is now the result of the *Wick theorem* for the harmonic Hamiltonian (A.8):

$$D_V(T, h) \equiv \left\langle \left( \frac{1}{V} \sum_{l \in \Lambda} Q_l^2 - \left\langle \frac{1}{V} \sum_{l \in \Lambda} Q_l^2 \right\rangle_{H_\Lambda(c_\Lambda, h)} \right)^2 \right\rangle_{H_\Lambda(c_\Lambda, h)} = \frac{2}{V^2} \sum_{k \in \Lambda^*} \left\{ \frac{\lambda}{2\Omega_k(c_\Lambda)} \coth \frac{1}{2} \beta\lambda\Omega_k(c_\Lambda) \right\}^2 + \frac{2}{V} \left( \frac{h^2}{\Delta^2(c_\Lambda)} \right)^2 \tag{A.16}$$

Now we have to distinguish two cases: (a) $a + 2W'(c \geq 0) > 0$ and (b) $a + 2W'(c)$ is a *monotonic increasing* function of $\mathbb{R}^1_+$ [see (ii) of (A.2)] with unique zero at $c^* > 0$.

(a) In this case the gap $\Delta(c) > 0$ for all $c \geq 0$. Hence the limit in (A.15) exists and

$$c(T, h) = \frac{h^2}{\Delta^2(c(T, h))} + \frac{1}{(2\pi)^d} \int_{\mathfrak{B}_d} d^d k \, \frac{\lambda}{2\Omega_k(c(T, h))} \coth \frac{1}{2} \beta\lambda\Omega_k(c(T, h)) \tag{A.17}$$

where $\mathfrak{B}_d = \mathsf{X}_{\alpha=1}^{d} [-\pi, \pi]$. For the same reason, i.e., $\Delta(c_\Lambda(T, h)) > 0$, one gets, by (A.16),

$$\lim_V D_V(T, h) = 0 \tag{A.18}$$

for any $T \geqslant 0$ and $h \in \mathbb{R}^1$.

(b) In this case $\Delta(c^*) = 0$. Hence, the solution of Eq. (A.15) (see Section 3 for details) exists and $c_\Lambda(T, h) > c^*$; moreover, for $h \neq 0$ one gets that $\lim_V c_\Lambda(T, h) = c(T, h) > c^*$ for $h \neq 0$ and any $T \geqslant 0$. Therefore, again $\Delta(c(T, h)) > 0$ and, as a consequence, we get (A.18) for $h \neq 0$. This means that we prove (A.9) in the form [cf. (A.14)]

$$\begin{aligned} f(T, h \neq 0) &= \lim_V f_V[H_\Lambda(h \neq 0)] \\ &= \frac{1}{\beta} \frac{1}{(2\pi)^d} \int_{\mathfrak{B}_d} d^d k \ln \left[ 2 \operatorname{sh} \frac{1}{2} \beta\lambda\Omega_k(c(T, h)) \right] \\ &\quad - \frac{1}{2} \frac{h^2}{\Delta^2(c(T, h))} + [W(c(T, h)) - c(T, h)\, W'(c(T, h))] \end{aligned} \tag{A.19}$$

where $c = c(T, h)$ is the solution of Eq. (A.17) for $h \neq 0$.

The free energy densities $f_V[H_\Lambda(h)]$ are convex functions of the variable $h \in \mathbb{R}^1$ as well as the limit $f(T, h)$. Therefore, we define $f(T, h = 0)$ in (A.9) and (A.19) by continuity:

$$f(T, h = 0) = \lim_{h \to 0} \lim_V f_V[H_\Lambda(h)] \quad \blacksquare$$

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## REFERENCES

1. A. Z. Patashinskii and V. I. Pokrovskii, *Fluctuation Theory of Phase Transitions* (Pergamon Press, Oxford, 1979); G. L. Sewell, *Quantum Theory of Collective Phenomena* (Clarendon Press, Oxford, 1986).
2. K. Alex Müller, W. Berlinger, and E. Tosatti, *Z. Phys. B Condensed Matter* **84**:277 (1991).
3. D. Goderis, A. Verbeure, and P. Vets, *Commun. Math. Phys.* **128**:533 (1990).
4. D. Goderis, A. Verbeure, and P. Vets, *Prob. Theory Related Fields* **82**:527 (1989).
5. D. Goderis, A. Verbeure, and P. Vets, *J. Stat. Phys.* **62**:759 (1991).
6. R. S. Ellis and C. M. Newman, *J. Stat. Phys.* **19**:149 (1978).
7. M. Fannes, A. Kossakowski, and A. Verbeure, *J. Stat. Phys.* **65**:801 (1991).
8. S. Stamenković, N. S. Tonchev, and V. A. Zagrebnov, *Physica* **145A**:262 (1987).
9. J. L. van Hemmen and V. A. Zagrebnov, *J. Stat. Phys.* **53**:835 (1988).

10. N. M. Plakida and N. S. Tonchev, *Theor. Math. Phys.* **63**:504 (1985).
11. A. Verbeure and V. A. Zagrebnov, Preprint-KUL-TF-91/42, *Phys. Rev. Lett.*, submitted.
12. A. D. Bruce and K. A. Cowley, *Structural Phase Transitions* (Taylor & Francis, London, 1981).
13. M. Fannes and A. Verbeure, *Commun. Math. Phys.* **55**:125 (1977); **57**:165 (1977).
14. O. Bratteli and D. W. Robinson, *Operator Algebras and Quantum Statistical Mechanics*, Vol. I (Springer-Verlag, New York, 1979).
15. K. Hepp and E. H. Lieb, *Helv. Phys. Acta* **46**:573 (1974).
16. A. Verbeure, Phonons limit and phonon dynamics, in *Proceedings of the 3rd Locarno International Conference "Stochastic Processes—Geometry and Physics"* (June 1991).
17. J. G. Brankov, N. S. Tonchev, and V. A. Zagrebnov, *Theor. Math. Phys.* **66**:72 (1986).
18. N. Angelescu and V. A. Zagrebnov, *J. Stat. Phys.* **41**:323 (1985).
19. M. E. Fisher and V. Privman, *Commun. Math. Phys.* **103**:527 (1986).
20. F. D. Walls, *Nature* **306**:141 (1983).
21. K. A. Müller, in *Nonlinear Phenomena at Phase Transition and Instabilities*, T. Riste, ed. (Plenum Press, New York, 1982).