Journal of Statistical Physics, Vol. 79, Nos. 1/2, 1995

Dynamics of Quantum Fluctuations in an Anharmonic Crystal Model

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Received June 13, 1994

For a model given previously by the authors describing a structural phase transition we compute the q-mode critical fluctuations of momentum and displacement as a function of the critical temperatures, the wave vector q, and a fading-out external field. An explicit dependence on the rates of fading out is obtained. In order to define the critical fluctuation operators we prove a reconstruction theorem, which is of model-independent value. Finally we study the critical spectrum and get rigorous results on the soft modes and the central peak.

KEY WORDS: Quantum fluctuation operators; order parameter; dynamics; critical line; phonon spectrum; soft modes; central peak problem.

1. INTRODUCTION

This is the second paper, following ref. 1, in which we study the critical fluctuations in an exactly soluble model for a quantum anharmonic crystal. The model and its thermodynamic properties are studied in refs. 2–4; it describes a structural phase transition.[5] More precisely, this model is a lattice phonon model consisting of an anharmonic crystal in which one-site anharmonicity terms are treated in its quantum spherical approximation. The model has a combination of short-range interactions and long-range interactions of the spherical type. It shows spontaneous symmetry breaking and the order parameter is the displacement from the lattice equilibrium position.

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0022-4715/95/0400-0377$07.50/0

The fluctuations on the critical line in the phase diagram are considered in ref. 1 with a special eye on the specific quantum nature of these fluctuations. In particular a new phenomenon is discovered, namely the squeezing of the momentum fluctuation operator, which forms a canonical pair with the critical displacement fluctuation operator. This happens at $T_c = 0$, which can be considered as a pure quantum phase transition.

In this paper we deal with further properties of the critical fluctuations. Recently[6] we computed the q-mode magnetization fluctuations as a function of the temperature, the wave vector q, and a fading-out external field for the Curie–Weiss model. Even for the most trivial model new classes of probability distributions are obtained which are generated by the external field. New critical behavior is obtained in terms of the rate of fading out of the field. By taking a particular long-wavelength limit ($q \to 0$) one obtains also interesting rigorous information about the magnetic susceptibility. In Section 3 of this paper we derive analogous results for the anharmonic quantum crystal model. The critical exponents of the displacement and momentum fluctuations are computed as a function of the rate of fading out of the external field in the long-wavelength limit. We find critical behavior in terms of both rates of decrease with the volume.

Section 3 contains also a reconstruction theorem defining these fluctuations as operators on a Hilbert space. This is useful in order to consider the quantum nature of fluctuations. In the case of normal fluctuations, it is proved that these fluctuations are representations of a Bose field.[7,8] Here we extend this result to critical abnormal fluctuations. These results have a model-independent value.

Finally, in Section 4, we start with the study of the dynamics of the algebra of fluctuation operators. A rigorous derivation is given of the phonon spectrum not only for the case that the wave vector $q \neq 0$, but also in the long-wavelength limit $q \to 0$. We derive some results about the soft modes and the so-called central peak problem.[5]

2. THE MODEL

Let $\mathscr{H} = L^2(\mathbb{R})$ and $\mathbb{Z}^d$ be the d dimensional cubic lattice; let Q and P be the usual canonical observables of multiplication and differentiation on $\mathscr{H}$ such that $[Q, P] = i$ ($\hbar = 1$). For each finite volume Λ of $\mathbb{Z}^d$, the model Hamiltonian is given by[2,3]

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

where $V = \# \Lambda$, $h_l \in \mathbb{R}$,

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

and $\{Q_l, P_l\}$ is a copy of $\{Q, P\}$ at the site $l \in \mathbb{Z}^d$; the potential ϕ is supposed to be of finite range and the term W is meant to include the one-site anharmonicity. For example, we take here $W(x) = \frac{1}{2} b \exp(-\eta x)$; $b, \eta > 0$ and b sufficiently large.[2] The model has been introduced in order to describe structural phase transitions in the self-consistent phonon framework.[5]

In this section we follow closely the presentation of ref. 1.

The model is soluble in the sense that for all temperatures the free energy density and all thermal averages can be calculated. Take for Λ the hypercube Λ with periodic boundary conditions

$$\Lambda = \left\{ l \in \mathbb{Z}^d \;\middle|\; -\frac{N_\alpha}{2} < l_2 \leqslant \frac{N_\alpha}{2};\ \alpha = 1, ..., d \right\}$$

and denote the dual volume

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

In the thermodynamic limit $\Lambda \to \mathbb{Z}^d$, the model is described by the effective Hamiltonian

$$H_\Lambda^e = T_\Lambda + W'(c_\Lambda) \sum_{l \in \Lambda} Q_l^2 - \sum_{l \in \Lambda} h_l Q_l \tag{2.2}$$

where c_Λ is determined by the self-consistency equation

$$c_\Lambda = \left\langle \frac{1}{V} \sum_{l \in \Lambda} Q_l^2 \right\rangle_{H^e} \tag{2.3}$$

The notation $\langle \cdot \rangle_{H^e}$ is used for the thermal average corresponding to the effective Hamiltonian (2.2). The essential property of this state is that it is a generalized free state. It is completely characterized by the one- and two-point functions. Moreover, because of the time-reversal invariance, the state is characterized by the expectation values

$$\langle Q_l \rangle_{H^e}, \qquad \langle Q_l, Q_{l'} \rangle_{H^e}, \qquad \langle P_l, P_{l'} \rangle_{H^e}$$

If the external field $h = 0$, then the model 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 invented in order to describe the phenomenon of the spontaneous breaking of this symmetry and of the softening of the phonon mode. One considers first $h \neq 0$ and then discusses the limit $h \to 0$.

The study of the phase diagram of the model is reduced to the study of the solutions of Eq. (2.3) in the thermodynamic limit $\Lambda \to \mathbb{Z}^d$ and in the limit $h \to 0$. Equation (2.3) becomes the following equation for the order parameter $c = \lim_\Lambda c_\Lambda$:

$$c = \rho + I_d(c, T, \lambda) \tag{2.4}$$

where, for $h_l = h$,

$$\rho = \lim_\Lambda \left[\frac{1}{V} \frac{\lambda}{2[\Delta(c_\Lambda)]^{1/2}} \coth \frac{\beta\lambda[\Delta(c_\Lambda)]^{1/2}}{2} + \frac{h^2}{\Delta^2(c_\Lambda)} \right]$$

$$I_d(c, T, \lambda) = \frac{\lambda}{(2\pi)^d} \int_{\mathscr{B}_d} dq \frac{\coth[\beta\lambda\Omega_q(c)/2]}{2\Omega_q(c)}$$

with

$$\mathscr{B}_d = \{q \in \mathbb{R}^d \mid |q_\alpha| \leqslant \pi\}$$

$$\lambda = \frac{1}{\sqrt{m}}$$

$$\Omega_q^2(c) = \omega_q^2 + \Delta(c)$$

$$\Delta(c) = a + 2W'(c)$$

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

and $\tilde{\phi}$ is the Fourier transform of the interaction ϕ_l.

The stability of the model is expresed by $\Omega_q^2(c) \geqslant 0$ for all $c \geqslant 0$. Define

$$c^* = \inf\{c \mid c \geqslant 0; \Delta(c) \geqslant 0\} \tag{2.5}$$

Then $\Delta(c^*) = 0$. Hence the domain of the order parameter $c = c(T, \lambda)$ as a solution of (2.4) is the interval $[c^*, \infty)$.

For fixed c^*, i.e., for a fixed potential W and for $h_l = h = 0$, the equation

$$c^* = I_d(c^*, T, \lambda) \tag{2.6}$$

defines a unique curve $\lambda_c(T)$ or $T_c(\lambda)$ separating the (T, λ) plane into two disjoint parts. In terms of the temperature, if $T > T_c(\lambda)$, then $\rho = 0$ in (2.4); this is the one-phase region. If $T < T_c(\lambda)$, then $\rho > 0$ in (2.4); this is the two-phase region, where the $\mathbb{Z}^2$ symmetry is spontaneously broken, and one has

$$\langle Q_0 \rangle_{\pm} = \lim_{h \to \pm 0} \lim_{\Lambda} \frac{1}{V} \left\langle \sum_{l \in \Lambda} Q_l \right\rangle_{H^c} \neq 0$$

In this paper we discuss the fluctuations of Q_l and P_l on the critical line $T_c(\lambda)$.

3. CRITICAL FLUCTUATION OPERATORS

As far as our model (2.2)–(2.3) is concerned, the basic observables are the local displacements $Q = \{Q_l\}$ and the conjugate momenta $P = \{P_l\}$. Moreover, these observables are also left globally invariant by the dynamics (2.2). Therefore we will consider the fluctuation operators of displacement and momentum on the critical line, together with its dynamics. The dynamics is postponed to the next section.

The local fluctuation operators in the q-mode, $q \in \mathscr{B}_d$, are defined by

$$F^q_{\delta,\Lambda}(Q) = \frac{1}{V^{1/2+\delta}} \sum_{l \in \Lambda} (Q_l - \langle Q_l \rangle_{H^c}) \cos q \cdot l \tag{3.1}$$

$$F^q_{\delta',\Lambda}(P) = \frac{1}{V^{1/2+\delta'}} \sum_{l \in \Lambda} (P_l - \langle P_l \rangle_{H^c}) \cos q \cdot l \tag{3.2}$$

The problem is to give a meaning to the limits

$$\lim_{\Lambda} F^q_{\delta,\Lambda}(Q) \equiv F^q_\delta(Q) \qquad \text{and} \qquad \lim_{\Lambda} F^q_{\delta',\Lambda}(P) \equiv F^q_{\delta'}(P) \tag{3.3}$$

which we simply call the fluctuation operators.

First of all we determine the parameters δ and δ' such that the variances of the operators exist and are not trivial, i.e., such that

$$0 < \lim_{\Lambda} \langle F^q_{\delta,\Lambda}(Q)^2 \rangle_{H^c} < \infty \tag{3.4}$$

$$0 < \lim_{\Lambda} \langle F^q_{\delta',\Lambda}(P)^2 \rangle_{H^c} < \infty \tag{3.5}$$

If $\delta = \delta' = 0$, then the displacement as well as the momentum will be called *normal fluctuation operators*. If $\delta \neq 0$ and/or $\delta' \neq 0$ they will be called *critical* or *abnormal*. For this model it will turn out that in all situations $\delta + \delta' \geqslant 0$. Therefore we will limit ourselves here to this situation in developing the mathematics in order to give a mathematical meaning to the fluctuation operators (3.3).

In ref. 1 we considered the fluctuations (3.2) and (3.2) also on the critical line $T=T_c(\lambda)$, but for $h=0$ and $q=0$. Also, we did not go into the details of the mathematics in order to give a full definition of the limiting fluctuation operators. Therefore our objective here is to fill in this gap and also to scrutinize the properties of the fluctuation operators in the limits of a fading-out field $h\to 0$ and of a wave vector $q\to 0$.

Theorem 3.1 (Central Limit Theorem). Suppose that δ and δ' are given such that (3.4) and (3.5) are satisfied. For $T=T_c(\lambda)\geqslant 0$, then for all h and q the distributions of the displacement and the momentum are Gaussian and given by

$$\lim_{\Lambda} \langle \exp i\lambda F^q_{\delta,\Lambda}(Q)\rangle_{H^c} = \exp\left\{-\frac{\lambda^2}{2}\lim_{\Lambda}\langle F^q_{\delta,\Lambda}(Q)^2\rangle_{H^c}\right\}$$

$$\lim_{\Lambda} \langle \exp i\lambda F^q_{\delta',\Lambda}(P)\rangle_{H^c} = \exp\left\{-\frac{\lambda^2}{2}\lim_{\Lambda}\langle F^q_{\delta',\Lambda}(P)^2\rangle_{H^c}\right\}$$

Proof. Consider the Hamiltonian H^c_Λ and the Fourier transforms: for $k\in\Lambda^*$,

$$Q(k)=\frac{1}{\sqrt{V}}\sum_{l\in\Lambda} Q_l e^{-ik\cdot l}, \qquad P(k)=\frac{1}{\sqrt{V}}\sum_{l\in\Lambda} P_l e^{-ik\cdot l}$$

Then

$$H^c_\Lambda = \sum_{k\in\Lambda^*} H^c_\Lambda(k)$$

where

$$H^c_\Lambda(k)=\frac{1}{2m}P(k)\,P(-k)+\frac{1}{2}m\tilde{\Omega}^2_k(c)\,Q(k)\,Q(-k)$$
$$-\frac{1}{2}\left[Q(k)\,h(-k)+Q(-k)\,h(k)\right]$$

with

$$h(-k)=\frac{1}{\sqrt{V}}\sum_{l\in\Lambda} h_l e^{ik\cdot l}$$

$$m\tilde{\Omega}^2_k(c)=\Omega^2_k(c)$$

Remark that

$$[H^{\mathrm{c}}_{\Lambda}(k), H^{\mathrm{c}}_{\Lambda}(k')] = 0$$

$$F^{q}_{\delta,\Lambda}(Q) = \frac{1}{2V^{\delta}} \{Q(q) + Q(-q) - \langle Q(q) + Q(-q) \rangle_{H^{\mathrm{c}}}\}$$

with the same for the P-fluctuation, and that H^{c}_{Λ} is a function at most quadratic in the $Q(k)$ and $P(k)$, such that the computation of the Q- and P-distributions become a one-mode computation in a quasi-free state $\langle \cdot \rangle_{H^{\mathrm{c}}}$. The result is obvious. ∎

This central limit theorem settles the problem of the sense in which the limits in (3.3) should be taken. Remark that these limits depend on the sequence $\Lambda \to \mathbb{Z}^d$ of equilibrium states one is taking. This dependence is one of the issues of this paper; see further. But we will first characterize the limits $F^{q}_{\delta}(Q)$ and $F^{q}_{\delta'}(P)$ of (3.3) as well-defined mathematical objects. In order to do that we use a specific reconstruction theorem, an extension of the one proved in ref. 7 for the case of normal fluctuations.

Consider the real two-dimensional vector space H generated by the operators Q and P on $\mathscr{L}^2(\mathbb{R})$, and the symplectic form σ_q defined for all $q \in \mathscr{B}_d$ and $\delta + \delta' \geqslant 0$ by

$$\sigma_q(Q, P) = \begin{cases} a(q) & \text{if } \delta + \delta' = 0 \\ 0 & \text{if } \delta + \delta' > 0 \end{cases} \tag{3.6}$$

where

$$a(q) = \lim_{\Lambda} \frac{1}{V} \sum_{l \in \Lambda} \cos^2 q \cdot l = \begin{cases} \frac{1}{2} & \text{if } q \neq 0 \\ 1 & \text{if } q = 0 \end{cases}$$

and

$$\sigma_q(Q, Q) = \sigma_q(P, P) = 0$$

Remark that in fact for $A = \alpha Q + \beta P$, $B = \alpha' Q + \beta' P$, $\alpha, \alpha', \beta, \beta' \in \mathbb{R}$,

$$\sigma_q(A, B) = i(\beta\alpha' - \alpha\beta') \lim_{\Lambda} \langle [F^{q}_{\delta,\Lambda}(Q), F^{q}_{\delta',\Lambda}(P)] \rangle_{H^{\mathrm{c}}}$$

Denote by $\mathscr{W}(H, \sigma_q)$ the Weyl algebra[6] of the canonical commutation relations generated by the Weyl operators $\{W(A) \mid A \in H\}$, satisfying the product rule

$$W(A)\, W(B) = W(A + B) \exp -\frac{i}{2} \sigma_q(A, B) \tag{3.7}$$

We have the following theorem.

Theorem 3.2 (Reconstruction Theorem). For each $A = \alpha Q + \beta P \in H$ denote

$$F^q_\Lambda(A) = \alpha F^q_{\delta, \Lambda}(Q) + \beta F^q_{\delta', \Lambda}(P)$$

Then the limits

$$\lim_\Lambda \langle \exp iF^q_\Lambda(A) \rangle_{H^c}$$

defined in Theorem 3.1 define a quasi-free state ω_{s_q} of $\mathscr{W}(H, \sigma_q)$:

$$\omega_{s_q}(W(A)) = \exp - \tfrac{1}{2} s_q(A, A)$$

where

$$s_q(A, A) = \alpha^2 \lim_\Lambda \langle F^q_{\delta, \Lambda}(Q)^2 \rangle_{H^c} + \beta^2 \lim_\Lambda \langle F^q_{\delta', \Lambda}(P)^2 \rangle_{H^c}$$

Proof. The existence of the quasi-free state ω_s follows from Theorem 3.1, namely the Gaussian form of the distribution, and from Schwartz' inequality expressed in the form

$$\tfrac{1}{4} |\sigma_q(A, B)|^2 \leqslant s_q(A, A)\, s_q(B, B)$$

(see, e.g., ref. 9). This proves the statement. ∎

This theorem characterizes the limiting fluctuation operators (3.3). The state ω_{s_q} on the CCR-algebra $\mathscr{W}(H, \sigma_q)$ determines by the GNS construction a representation π on a Hilbert space $\mathscr{H}$ and a cyclic vector Ω such that

$$\omega_{s_q}(W(A)) = (\Omega, \pi(W(A))\Omega) = \exp - \tfrac{1}{2} s_q(A, A)$$

Remark that the state ω_{s_q} is a regular state, so that the existence of Bose fields is guaranteed:

$$\pi(W(A)) = \exp iF^q(A)$$

where

$$F^q(A) = \begin{cases} F^q_\delta(Q) & \text{if } A = Q \\ F^q_{\delta'}(P) & \text{if } A = P \end{cases}$$

are the Bose fields on $\mathscr{H}$ satisfying the commutation relation

$$[F^q_\delta(Q), F^q_{\delta'}(P)] = i\sigma_q(Q, P) \tag{3.8}$$

where $\sigma_q(Q, P)$ is given by (3.6).

Now we identify in a mathematically rigorous way the fluctuation operators by means of Theorems 3.1 and 3.2 up to the solution of (3.4) and (3.5), which should fix the values of δ and δ'. Now we proceed with the explicit computation of these indices on the critical line. In particular we consider their dependence on the limits $h \to 0$ and $q \to 0$.

The self-consistency equation (2.3) plays of course an essential role in this computation. A straightforward computation yields for (2.3)

$$c_\Lambda = \frac{h^2}{\Delta^2(c_\Lambda)} + \frac{1}{V}\frac{\lambda}{2[\Delta(c_\Lambda)]^{1/2}} \coth \frac{\beta_c \lambda}{2} [\Delta(c_\Lambda)]^{1/2}$$
$$+ \frac{1}{V} \sum_{\substack{k \in \Lambda^* \\ k \neq 0}} \frac{\coth \frac{1}{2}\beta_c \lambda \Omega_k(c_\Lambda)}{2\Omega_k(c_\Lambda)} \tag{3.9}$$

where $\Omega_k(c_\Lambda) = [\Delta(c_\Lambda) + \omega_k^2]^{1/2}$.

Remark that c_Λ depends on $T_c(\lambda)$ and on h, that for short-range interactions one has $\omega_k \simeq s \cdot k + O(k^2)$ for $k \to 0$, and that $\lim_{h \to 0} \lim_\Lambda c_\Lambda(T_c, h) = 0$.

Using the diagonalization of H_Λ^c used in the proof of Theorem 3.1, one computes straightforwardly that

$$\langle F_{\delta,\Lambda}^q(Q)^2 \rangle_{H^c} = \frac{1}{V^{2\delta}} \frac{\lambda}{2\Omega_q} \coth \frac{\lambda \beta_c(\lambda) \Omega_q}{2} \tag{3.10}$$

$$\langle F_{\delta',\Lambda}^q(P)^2 \rangle_{H^c} = \frac{1}{V^{2\delta'}} \frac{\lambda m}{2} \Omega_q \coth \frac{\lambda \beta_c(\lambda) \Omega_q}{2} \tag{3.11}$$

Theorem 3.3. Suppose that $T_c(\lambda) > 0$; then one gets the following results for δ and δ' such that (3.5) and (3.5) are satisfied:

(i) If $q \neq 0$, then $\delta = \delta' = 0$.

(ii) If $h \neq 0$, then again $\delta = \delta' = 0$.

(iii) If $q = 0$ and $h \to 0$, such that $h = \hat{h}/V^\alpha$, $\alpha \geqslant 0$, one gets

$$.\delta_{d=3} = \begin{cases} \frac{2}{5}\alpha & \text{for } 0 \leqslant \alpha < \frac{5}{6} \equiv \alpha_c \quad (d=3) \\ \frac{1}{3} & \text{for } \frac{5}{6} \leqslant \alpha \end{cases}$$

$$\delta_{d \geqslant 4} = \begin{cases} \alpha/3 & \text{for } 0 \leqslant \alpha < \frac{3}{4} \equiv \alpha_c \quad (d=4) \\ \frac{1}{4} & \text{for } \frac{3}{4} \leqslant \alpha \end{cases}$$

and $\delta' = 0$.

(iv) If $h=0$ and $q\to 0$, such that $q=\hat{q}/V^{\gamma}$, $\gamma\geqslant 0$, then

$$\delta_{d=3}=\begin{cases}\frac{1}{3} & \text{for } \frac{1}{3}\leqslant\gamma\\ \gamma & \text{for } 0\leqslant\gamma<\frac{1}{3}\equiv\gamma_c\end{cases}\quad (d=3)$$

$$\delta_{d\geqslant 4}=\begin{cases}\frac{1}{4} & \text{for } \frac{1}{4}\leqslant\gamma\\ \gamma & \text{for } 0\leqslant\gamma<\frac{1}{4}\equiv\gamma_c\end{cases}\quad (d\geqslant 4)$$

and $\delta'=0$.

(v) If now $h=\hat{h}/V^{\alpha}$ and $q=\hat{q}/V^{\gamma}$, then

$$\delta=\min\{\eta,\gamma\}$$

where

$$\eta_{d=3}=\begin{cases}\frac{2}{5}\alpha & \text{for } 0\leqslant\alpha<\frac{5}{6}\\ \frac{1}{3} & \text{for } \frac{5}{6}\leqslant\alpha\end{cases}$$

$$\eta_{d\geqslant 4}=\begin{cases}\frac{1}{3}\alpha & \text{for } 0\leqslant\alpha<\frac{3}{4}\\ \frac{1}{4} & \text{for } \frac{3}{4}\leqslant\alpha\end{cases}$$

and $\delta'=0$.

Proof. Consider first the easy case of the index δ' in the q-mode momentum fluctuation operator. Because of the formula (3.11), the cases (i)–(v) reduce to two cases $\Omega_q>0$ or $\lim_{q\to 0}\Omega_q=0$. In both cases there is only one solution δ' for the conditions (3.5) to hold, that is, $\delta'=0$.

Consider now the q-mode displacement fluctuation operator. If $q\neq 0$, then $\omega_q>0$, and the limit (3.10) will be nontrivial only if $\delta=0$.

This proves (i).

If $h\neq 0$, then it follows from (3.9) that $\lim_{\Lambda} c_{\Lambda}>c^*$ [see (2.5)], i.e., $\lim_{\Lambda}\Delta(c_{\Lambda})>0$. Therefore (3.5) has only the solution $\delta=0$. This proves (ii).

If we take $h=\hat{h}/V^{\alpha}$, $\alpha\geqslant 0$, then Eq. (3.9) becomes

$$c_{\Lambda}=\frac{\hat{h}^2}{V^{2\alpha}\Delta^2(c_{\Lambda})}+\frac{1}{V}\frac{\lambda}{2[\Delta(c_{\Lambda})]^{1/2}}\coth\frac{\beta_c\lambda}{2}[\Delta(c_{\lambda})]^{1/2} +\frac{1}{V}\sum_{\substack{k\in\Lambda^*\\ k\neq 0}}\frac{\coth\frac{1}{2}\beta_c\lambda\Omega_k(c_{\Lambda})}{2\Omega_k(c_{\Lambda})} \tag{3.12}$$

At $T_c(\lambda)$ one has that $\lim_{\Lambda} c_{\Lambda}(T_c,\hat{h}/V^{\alpha})=0$. Therefore one can follow the argumentation as in the proof of Proposition 4.3 of ref. 1, but with the modification due to the presence of the first term in the right-hand side of (3.9):

$$\begin{aligned} c_\Lambda - c^* &+ [c^* - I_d(c_\Lambda, T_c, \lambda)] \\ &+ \left[I_d(c_\Lambda, T_c, \lambda) - \frac{1}{V} \sum_{k \neq 0} \frac{\lambda}{2\Omega_k(c_\Lambda)} \coth \frac{1}{2} \beta_c \lambda \Omega_k(c_\Lambda) \right] \\ &= \left(\frac{\hat{h}}{V^\alpha \Delta(c_\Lambda)} \right)^2 + \frac{1}{V} \frac{\lambda}{2[\Delta(c_\Lambda)]^{1/2}} \coth \frac{\beta_c \lambda}{2} [\Delta(c_\Lambda)]^{1/2} \\ &\simeq \left(\frac{\hat{h}}{V^\alpha \Delta(c_\Lambda)} \right)^2 + \frac{T_c(\lambda)}{V \Delta(c_\Lambda)} \end{aligned} \tag{3.13}$$

for large V. Therefore, if $\alpha \geqslant 1$, the behavior is determined by the second term and we get the result of ref. 1, corresponding to the case $h = 0$. Hence we limit here our considerations to the case $\alpha < 1$. Using the asymptotics

$$c^* - I_d(c_\Lambda, T_c, \lambda) \simeq \begin{cases} \Delta(c_\Lambda)^{1/2}, & d = 3 \\ \Delta(c_\Lambda) \ |\ln \Delta(c_\Lambda)|, & d = 4 \\ \Delta(c_\Lambda), & d > 4 \end{cases} \tag{3.14}$$

for $\Delta(c_\Lambda) \to 0$,[1] one finds the results (iii).

If now $h = 0$ and $q = \hat{q}/V^\gamma$, $\gamma \geqslant 0$, then the proper choice of the exponent δ reduces to considering (3.9) with $h = 0$. From ref. 1, one gets that $\Delta(c_\Lambda) \simeq V^{-2/3}$ $(d = 3)$, $\Delta(c_\Lambda) \simeq (V^{1/2} \ln V)^{-1}$ $(d = 4)$, and $\Delta(c_\Lambda) \simeq V^{-1/2}$ $(d > 4)$ for $V \to \infty$. One finds the result (iv).

Finally, consider now the case $q = \hat{q}/V^\gamma$ and $h = \hat{h}/V^\alpha$, $\alpha \geqslant 0$, $\gamma \geqslant 0$. From (3.10) and the definition of Ω_q, it is clear that the exponent δ is determined by the slowest of the two asymptotics $\Delta \to 0$ or $\omega_q^2 \to 0$. Let $\Delta(c_\Lambda) \simeq V^{-2\eta}$; one gets grom (3.13) that $\eta = \delta_d$, where δ_d is as given in (iv). Then combining this with the results of (iv), one gets (v). ∎

There are a number of remarks to make.

In the theorem we proved that the momentum fluctuation operator is always Gaussian and normal on the critical line for $T_c > 0$. On the other hand, the displacement fluctuation operator is Gaussian and normal if $q \neq 0$ and/or $h \neq 0$. This behavior for $h \neq 0$ was expected. The case $q \neq 0$ is the first quantum mechanical result analogous to what was called "fluctuations within the fluctuating field are Gaussian"[11] in the case of the Curie–Weiss model. For a complete understanding of this phenomenon in this classical model see ref. 6, where it is proved that nontrivially modulated $(q \neq 0)$ fluctuations are always Gaussian and normal.

The theorem yields also results if one considers particular fadings out of the external field in the form $h = \hat{h}/V^{\alpha}$. This means that the external field tends to zero when the volume increases to infinity. The theorem shows the phenomenon that the critical exponent depends on the parameter α if $\alpha < \alpha_c(d)$, where $\alpha_c(d)$ does appear as another critical parameter which depends on the dimension. If the external field drops off too fast, i.e., $\alpha \geqslant \alpha_c(d)$, then no effect coming from the presence of the field is seen. It is as if there was no field. On the other hand, if the field is more persistently present, it influences very much the volume level at which the fluctuations do appear. If $0 < \alpha < \alpha_c(d)$ all fluctuations are Gaussian, but abnormal or critical. In principle the same phenomena happen if $q \to 0$, and there is a competition between the $q \to 0$ and the $h \to 0$. If one takes $q = \hat{q}/V^{\gamma}$, there is also a critical value $\gamma_c(d)$ for the exponent γ, such that the long-wavelength limit with a rate $0 < \gamma < \gamma_c(d)$ creates a dependence of the fluctuation abnormality δ on the rate γ. So far we have considered the results on the critical line for $T_c(\lambda) > 0$; it remains to consider the case $T_c(\lambda = \lambda_c) = 0$ for the pure quantum critical fluctuations.

Theorem 3.4. If $T_c(\lambda = \lambda_c) = 0$, then the displacement fluctuation operator has an abnormal Gaussian distribution with the exponent $\delta > 0$, depending on the rate α of the fading-out external field and on the rate γ determining the long-wavelength limit. On the other hand, the momentum fluctuation operator has a subnormal Gaussian distribution with exponent $\delta' = -\delta$.

Proof. The critical fluctuations at $T_c(\lambda_c) = 0$ are obtained as the $\lim_{\lambda \to \lambda_c} T_c(\lambda)$ of the corresponding ones at $T_c(\lambda < \lambda_c)$. Then the theorem follows from (3.11) yielding at $T_c(\lambda_c) = 0$

$$\langle F^q_{\delta,\Lambda}(Q)^2 \rangle_{H^c} \simeq \frac{1}{V^{2\delta}} \frac{\lambda_c}{2\Omega_q}$$

$$\langle F^q_{\delta',\Lambda}(P)^2 \rangle_{H^c} \simeq \frac{1}{V^{2\delta'}} \frac{\lambda_c m}{2} \Omega_q$$

From this it follows immediately that $\delta' = -\delta$ in all cases. It remains to look for, e.g., δ. But this is obtained analogously as in the proof of Theorem 3.3(v). We get straightforwardly

$$\delta = \min\left\{\rho, \frac{\gamma}{2}\right\}$$

where ρ is again determined by the self-consistency equation (3.9) or (3.12), (3.13), for $\beta = \infty$, and is given by

$$\rho_{d=2} = \begin{cases} \frac{1}{5}\alpha & \text{if } 0 \leqslant \alpha < \frac{5}{4} \equiv \tilde{\alpha}_c \quad (d=2) \\ \frac{1}{4} & \text{if } \frac{5}{4} \leqslant \alpha \end{cases}$$

$$\rho_{d \geqslant 3} = \begin{cases} \frac{1}{6}\alpha & \text{if } 0 \leqslant \alpha < 1 \equiv \tilde{\alpha}_c \quad (d \geqslant 3) \\ \frac{1}{6} & \text{if } 1 \leqslant \alpha \end{cases}$$

This proves the theorem. ∎

It is clear that the case $T_c(\lambda_c) = 0$ yields different exponents δ than in the case $T_c(\lambda < \lambda_c) > 0$. Nevertheless the exponents depend also on the rates of fading out of the external field as well as on the rate of the long-wavelength limit. As in ref. 1, we have the phenomenon of squeezing of the momentum fluctuation operator and a nontrivial commutation relation between the displacement and momentum fluctuation operators.

4. FLUCTUATION DYNAMICS, SOFT-MODE, AND CENTRAL PEAK PROBLEMS

In this section we consider the dynamics of the fluctuation operators $\{F^q(A) \mid A \in (H, \sigma_q)\}$ induced by the microscopic dynamics of the model (2.1) or rather (2.2).

The general setup of such a fluctuation dynamics is given in ref. 8 for normal fluctuations. Here we are mainly interested in the critical dynamics of our model, i.e., on the critical line.

For a local microscopic observable, say A, its time evolution is given by the Heisenberg equation

$$\alpha_t(A) = \lim_{\Lambda} e^{it[H_\Lambda, \cdot]} A$$

in integrated form or by

$$\frac{d}{dt} \alpha_t(A) = \lim_{\Lambda} i[H_\Lambda, \alpha_t(A)]$$

where the limit is taken in the norm or weak operator topology sense. Here we will use the dynamics defined by the effective Hamiltonian H_Λ^e, (2.2).

Following the general theory of ref. 8, this time evolution induces a dynamics of the fluctuation operator algebra defined by Theorem 3.2.

In particular we define the evolution $\tilde{\alpha}_t$ of the fluctuations by the formula

$$\begin{aligned}\tilde{\alpha}_t F^q(A) &= \lim_{\Lambda} F^q_\Lambda(e^{itH^c_\Lambda} A e^{-itH^c_\Lambda}) \\ &= \lim_{\Lambda} e^{itH^c_\Lambda} A e^{-itH^c_\Lambda} F^q_\Lambda(A)\, e^{-itH^c_\Lambda} \end{aligned} \tag{4.1}$$

where $\lim_\Lambda$ is in the sense of the Central Limit Theorem 3.1. Formula (4.1) can of course also be expressed in its differential form.

The first thing we have to check is whether Theorem 3.1 is valid in this case. It is indeed valid because of the particular situation of our model. The Hamiltonian H^c_Λ is nothing but a sum of local harmonic oscillator Hamiltonians such that for $A = Q$ or P, their time-evolved operators are again local. An explicit computation yields for $q \neq 0$

$$\tilde{\delta} F^q_\delta(Q) = \lim_{\Lambda} [H^c_\Lambda, F^q_{\delta,\Lambda}(Q)] = \frac{\lambda}{i\sqrt{m}} F^q_\delta(P) \tag{4.2}$$

$$\tilde{\delta} F^q_{\delta'}(P) = \lim_{\Lambda} [H^c_\Lambda, F^q_{\delta',\Lambda}(P)] = i\lambda\sqrt{m}\, \Omega^2_q(c)\, F^q_{\delta'}(Q) \tag{4.3}$$

where $\lim_\Lambda$ is taken in the sense of the Central Limit Theorem. We used the notation $\tilde{\delta}$ for $(d/i\,di)|_{t=0}$. It is clear that the dynamics $\tilde{\alpha}_t$ is given by $\tilde{\alpha}_t = \exp it\tilde{\delta}$, such that in Eq. (4.2) and (4.3) the fluctuations in the left-hand side exist. The whole problem of the analysis of these equations is now to use the results for the exponents δ and δ' derived in the previous section, and to find out what their values imply for the dynamics.

First of all there is the easy situation, dealing with all results of Theorems 3.3 and 3.4, yielding $\delta = \delta'$. This turns out to be the cases that $q \neq 0$ and/or $h \neq 0$, and then one has $\delta = \delta' = 0$.

Theorem 4.1. If $\delta = \delta'$, then the solution of (4.1) is given by

$$\begin{aligned}\tilde{\alpha}_t F^q_\delta(Q) &= (\exp it\tilde{\delta})\, F^q_\delta(Q) \\ &= F^q_\delta(Q) \cos[\lambda\Omega_q(c)t] + \frac{F^q_\delta(P)}{\lambda\Omega_q(c)} \sin[\lambda\Omega_q(c)t] \end{aligned} \tag{4.4}$$

and analogously for $F^q_\delta(P)$.

Proof. It is a straightforward consequence of (4.1)–(4.3) for $\delta = \delta'$. ∎

Remark that if $\delta = \delta' = 0$, then $\lambda\Omega_q(c)$ is a discrete point in the spectrum of $\tilde{\alpha}_t$; the eigenvectors are the normal fluctuation operators of displacement and momentum. This frequency coincides with the standard phonon frequency $\tilde{\Omega}_q$ for the q-mode phonons in the effective Hamiltonian H^e_Λ; here $\tilde{\Omega}_q = \Omega_q/\sqrt{m}$. This means that for this model of an anharmonic crystal, the transition to fluctuation modes for $q = 0$ reproduces the well-known phonon limit and phonon dynamics. It is clear that this result also holds for any q outside of the critical region, i.e., as far as the energy gap $\Delta(c)$ is strictly positive.

New interesting phenomena do appear on the critical line $T = T_c(\lambda)$ with $h = 0$.

Theorem 4.2. On the critical line $T_c(\lambda) \geqslant 0$ with $h = 0$, the zero-mode fluctuations are eigenfunctions of the dynamics $\tilde{\alpha}_t$ with zero frequency; in particular, one has

$$\tilde{\delta} F^0_\delta(Q) = 0 \qquad \text{and} \qquad \tilde{\delta} F^0_{\delta'}(P) = 0$$

where δ and δ' take the values determined in Theorem 3.3.

Proof. From Theorem 3.3 we learn that, for $q \to 0$ and $h \to 0$, the displacement fluctuation is always abnormal with critical exponent $\delta > 0$, whereas the momentum fluctuation is normal, i.e., $\delta' = 0$. Therefore one has always for all q that $F^q_\delta(P) = 0$. Then from (4.2) it follows immediately that $\tilde{\delta} F^0_\delta(Q) = 0$.

The analysis of Eq. (4.3) is more delicate because the fluctuation operator $F^0_0(Q)$ does not exist. For $q = 0$, Eq. (4.3) can be written as follows:

$$\tilde{\delta} F^0_0(P) = \lim_\Lambda \left\{ i\lambda \sqrt{m} \frac{\Delta(c_\Lambda)}{V^{1/2}} \sum_{l \in \Lambda} (Q_l - \langle Q_l \rangle_{H^e} \right\} \tag{4.5}$$

where the $\lim_\Lambda$ has to be understood as a central limit (see Theorem 3.1) with $h \to 0$. From the proof of Theorem 3.3(v) one gets that $\Delta(c_\Lambda) \simeq V^{-2\eta}$ and that $\delta = \eta > 0$ (here we are in the case $q = 0$ or formally $\gamma = \infty$). This means that the right-hand side of (4.5) behaves as $F^0_{2\delta,\Lambda}(Q)$, which vanishes in the limit Λ tending to infinity if $\delta > 0$, as is the case when $h \to 0$, with $\alpha > 0$. This settles the proof of the theorem for all critical temperatures $T_c(\lambda) > 0$.

On the other hand, if $T_c(\lambda_c) = 0$, by Theorem 3.4 one has $\delta = -\delta' > 0$. Therefore, Eq. (4.2) yields also $\tilde{\delta} F^0_\delta(Q) = 0$. But the analysis of Eq. (4.3) has to be based on the different behavior of the energy gap at $T_c(\lambda_c) = 0$; see proof of Theorem 3.4: for large V,

$$[\Delta(c_\Lambda)]^{1/2} \simeq \frac{1}{V^{2\delta}} \frac{\lambda_c}{2\langle F^0_\delta(Q)^2 \rangle_{H^e}}$$

Hence, using expression (4.3), analogous to (4.5), one gets

$$\tilde{\delta}F^0_{\delta'}(P) = \lim_{\Lambda} \left\{ \frac{i\lambda_c^2 \sqrt{m}}{4\langle F^0_\delta(Q)^2 \rangle^2_{H^c}} \frac{1}{V^{2\delta} V^{1/2+\delta}} \sum_l [Q_l - \langle Q_l \rangle_{H^c}] \right\}$$

$$= \lim_{\Lambda} \frac{i}{V^{2\delta}} \left(\frac{\lambda_c}{2\langle F^0_\delta(Q)^2 \rangle_{H^c}} \right)^2 F^0_{\delta,\Lambda}(Q) = 0$$

which proves the freezing of both fluctuations as operators also at $T_c(\lambda_c) = 0$. ∎

The equation $\tilde{\delta}F^0_\delta(Q) = 0$ is the mathematical expression of the so-called soft-mode phenomena known in the theory of the displacement structural phase transitions on the critical line.[5] Here the softening means that the evolution of the zero-mode displacement fluctuation on the critical line is frozen. We get also the freezing of the momentum fluctuation operator. Usually in the physicss literature this freezing of the evolution is treated formally by the argument that $\Omega_q \to 0$ for $q \to 0$. However, as can be concluded from Theorem 4.2, this simple procedure does not give very much information on the dynamics on the critical line, because we have to take into account that there $\delta \neq \delta'$ [see (4.5) and (4.6)]. Here we prove that we really have a zero-frequency mode.

We remarked above that $\{\tilde{\Omega}_q(c^*)\}_{q \neq 0}$ coincides with the usual phonon spectrum. Insofar as $\lim_{q \to 0} \tilde{\Omega}_q(c^*) = 0$, one can interpret zero as the limiting point, "soft mode," of the spectrum for the nonzero modes. A rigorous treatment of this point of view leads to an analysis in which the exponents δ and δ' depend on the wave vector $q \to 0$; see Theorems 3.3 and 3.4.

Finally, the analysis of Theorem 4.2 can also be looked upon from the point of view of the effective Hamiltonian (2.2). In that terminology, the result of Theorem 4.2 can be expressed as a rigorous treatment of the central peak problem[5] in our model.

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