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Quantum n-Vector Anharmonic Crystal II: Displacement Fluctuations

N. Angelescu,[1] A. Verbeure,[2] and V. A. Zagrebnov[3]

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Based on the $1/n$-expansion derived in a previous paper, the displacement fluctuations are analyzed in a quantum n-vector model of anharmonic crystal in the large n regime. It is shown that in the ferroelectric phase the $n \to \infty$ limit of the local fluctuation field has faster large-distance correlation decay than its Hartree–Fock approximation. Also, the critical exponent of the global displacement fluctuation is strictly smaller there than the Hartree–Fock exponent. In particular, the displacement fluctuations may be normal in the ferroelectric phase in spite of the Hartree–Fock prediction.

KEY WORDS: Quantum anharmonic crystal; large n-limit; large-distance correlations; fluctuations.

1. INTRODUCTION

In a previous paper[(1)] we considered a model of quantum anharmonic crystal with n-dimensional displacement operators for each oscillator (proposed in ref. 2), and we proved, under the assumption of isotropy of the (quartic anharmonic) one-body-, and (harmonic) two-body-, potentials, that the free energy and the equilibrium state $\langle \cdot \rangle_{N,n}$ of the model on a *finite lattice*, e.g., $\Lambda_N \subset \mathbf{Z}^d$ with $|\Lambda_N| = N^d$ sites, allow, for large number n of components, complete asymptotic expansions in powers of $1/n$. The leading term of those expansions coincide with the Hartree–Fock result, i.e., the $n = \infty$ limit state $\langle \cdot \rangle_N^{HF}$ is an infinite product of identical states of a scalar

[1] Department of Theoretical Physics, Institute of Atomic Physics, P.O. Box MG-6, Bucharest, Romania; e-mail: nangel@theor1.theory.nipne.ro.

[2] Instituut voor Theoretische Fysica, Katholieke Universiteit Leuven, Celestijnenlaan 200 D, B-3001 Leuven, Belgium; e-mail: andre.verbeure@fys.kuleuven.ac.be.

[3] Université de la Méditerranée and Centre de Physique Théorique, Luminy Case 907, F-13248 Marseille Cedex 9, France; e-mail: zagrebnov@cpt.univ-mrs.fr.

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harmonic oscillator model with a self-consistently defined Hamiltonian. However, for physically interesting quantities, such as fluctuations or susceptibilities, which involve all components, the $n=\infty$ result is different, in general, from the Hartree–Fock one, because the higher order terms of the $1/n$-expansion may sum up to nontrivial contributions in the limit. In the present work we point out that these higher order corrections imply, already in leading order in n, qualitative changes in the distribution of such observables in the equilibrium states of the *infinite crystal*, as compared to the Hartree–Fock prediction.

More precisely, our framework is the theory of quantum fluctuations, or quantum central limit theorem, as developed in ref. 3 applied to our situation, where the number of degrees of freedom goes to infinity already on account of $n \to \infty$. For any one-component observable, i.e., self-adjoint operator A acting in $L_2(\mathbf{R}^{\Lambda_N})$, its fluctuation in the equilibrium state $\langle \cdot \rangle_{N,n}$ of the n-component model on Λ_N is defined as:

$$F^{(N,n)}(A) = n^{-1/2} \sum_{\alpha=1}^{n} (A_\alpha - \langle A_\alpha \rangle_{N,n}) \tag{1.1}$$

where $A_\alpha = 1 \otimes \cdots \otimes A_\alpha \otimes \cdots \otimes 1$ is the copy of A acting on the α component in $\bigotimes_{\alpha=1}^{n} L_2(\mathbf{R}^{\Lambda_N})$. As $n \to \infty$, the restriction of the equilibrium state $\langle \cdot \rangle_{N,n}$ to the fluctuation operators $F^{(N,n)}(A)$ converges (in the sense of convergence of characteristic functions) to a quasifree state ω_N of a CCR (canonical commutation relation) algebra, $\mathscr{F}_N$, named the algebra of fluctuations. We denote this kind of convergence

$$\lim_{n \to \infty} F^{(N,n)}(A) = F^{(N)}(A) \in \mathscr{F}_N \tag{1.2}$$

Likewise, one can define the Hartree–Fock counterpart of this construction by replacing everywhere the exact state $\langle \cdot \rangle_{N,n}$ with the limit product state $\langle \cdot \rangle_N^{HF}$, i.e., consider the limits of the characteristic functions with respect to $\langle \cdot \rangle_N^{HF}$ of the operators:

$$\tilde{F}^{(N,n)}(A) = n^{-1/2} \sum_{\alpha=1}^{n} (A_\alpha - \langle A_\alpha \rangle_N^{HF}) \tag{1.1$'$}$$

In this way, one constructs a different quasifree state $\tilde{\omega}_N$ on a CCR algebra $\tilde{\mathscr{F}}_N$ of Hartree–Fock fluctuations. The corresponding limit is denoted

$$\lim_{n \to \infty} \tilde{F}^{(N,n)}(A) = \tilde{F}^{(N)}(A) \in \tilde{\mathscr{F}}_N \tag{1.2$'$}$$

In ref. 1 we considered the $1/n$-expansion for the fluctuations (1.1), (1.1′) in the cases $A = q_x$ (displacement), and $A = q_x^2$, (squared-displacement)

($x \in \Lambda_N$), and in particular calculated the explicit form of the leading term, i.e., showed that the limits $F^{(N)}(q_x)$ and $F^{(N)}(q_x^2)$ (respectively, $\tilde{F}^{(N)}(q_x)$ and $\tilde{F}^{(N)}(q_x^2)$) ($x \in \Lambda_N$) are distributed in ω_N (respectively, in $\tilde{\omega}_N$) as Gaussian vectors with covariance matrices $C_{x,y}^{(N)}$ and $D_{x,y}^{(N)}$ (respectively, $\tilde{C}_{x,y}^{(N)}$ and $\tilde{D}_{x,y}^{(N)}$). The formulae of ref. 1 will be reproduced in the new context (e.g., assuming translation invariance) in Section 2.

Here, we propose to show on an example that the thermodynamic limits ω and $\tilde{\omega}$ of the states ω_N and $\tilde{\omega}_N$ on the corresponding fluctuation algebras are qualitatively different in the many phase region. Namely, we define the (exact and Hartree–Fock) *local displacement fluctuation fields* in the thermodynamic limit as the limits $F(q_x)$ and $\tilde{F}(q_x)$ ($x \in \mathbf{Z}^d$) in finite volume distributions of the Gaussian vectors $F^{(N)}(q_x)$ and $\tilde{F}^{(N)}(q_x)$, respectively. The main result to be proved in Section 3 is essentially contained in the following

Theorem. In a pure phase in the many phase region, i.e., whenever

$$\lim_{h \searrow 0} \lim_{N, n \to \infty} \langle q_x^\alpha \rangle_{N,n} =: M > 0 \tag{1.3}$$

$F(q_x)$ and $\tilde{F}(q_x)$ ($x \in \mathbf{Z}^d$) are singular Gaussian fields with covariance operators

$$C_{x,y} := \omega(F(q_x)\, F(q_y)) \qquad \text{and} \qquad \tilde{C}_{x,y} := \tilde{\omega}(\tilde{F}(q_x)\, \tilde{F}(q_y)) \tag{1.4}$$

related at large distances by the relation

$$C_{x,y} \sim \frac{\beta}{2M^2} (\tilde{C}_{x,y})^2, \qquad |x-y| \to \infty \tag{1.5}$$

Remarks. 1. The large distance behaviour of $\tilde{C}_{x,y}$ is well studied (it is in fact the correlation function of a harmonic crystal) and known to obey the power law $|x-y|^{-d-2}$. While the latter clustering is non-summable in all dimensions d, Eq. (1.5) implies summable clustering of the "exact" local fluctuation field $F(q_x)$ (in particular, normal global displacement fluctuations) for $d > 4$.

2. An interpretation of the result above may be done in terms of longitudinal and transverse projections of the displacements. The displacement vector at a point x, $\vec{q}_x = (q_x^\alpha)_{\alpha=1,\dots,n} \in \mathbf{R}^n$ has, in view of the permutation symmetry, the expectation $\langle \vec{q}_x \rangle_{N,n}$ along the unit vector

$$\vec{e} = \frac{1}{\sqrt{n}} (1,\dots,1) \in \mathbf{R}^n \tag{1.6}$$

We fix one among the equivalent orthogonal directions, $\vec{e}_\perp$ ($\vec{e}_\perp^{\,2}=1$, $\vec{e}_\perp \cdot \vec{e}=0$), say

$$\vec{e}_\perp = \frac{\sqrt{n}}{\sqrt{n-1}}\,\vec{e}_1 - \frac{1}{\sqrt{n-1}}\,\vec{e} \tag{1.6$'$}$$

Then, $F^{(N,n)}(q_x)=(\vec{e}, \vec{q}_x - \langle \vec{q}_x \rangle_{N,n})$, i.e., $F(q_x)$ is in fact the field of deviations from its expectation of the projection of $\vec{q}_x$ along its expectation. On the other hand, it can be easily seen that $\tilde{F}^{(N,n)}(q_x)$ is distributed in the product state $\langle \cdot \rangle_N^{HF}$ like $q_x^1 - \langle q_x^1 \rangle_N^{HF}$, therefore it has for $n \to \infty$ the same distribution as $(\vec{e}_\perp, \vec{q}_x)$, e.g., with the choice (1.6′)

$$\begin{aligned}
q_x^1 - \langle q_x^1 \rangle_N^{HF} - (\vec{e}_\perp, \vec{q}_x)
&= \frac{\sqrt{n}}{\sqrt{n-1}} \left(\frac{1}{\sqrt{n}}\, F^{(N,n)}(q_x) + \langle q_x^1 \rangle_{N,n} - \langle q_x^1 \rangle_N^{HF} \right) \\
&\quad + \left(1 - \frac{\sqrt{n}}{\sqrt{n-1}}\right)(q_x^1 - \langle q_x^1 \rangle_N^{HF})
\end{aligned}$$

converges in distribution to 0 as a consequence of the convergence of $F^{(N,n)}(q_x)$.

3. The same asymptotics, as well as the relation (1.5) between longitudinal and transverse correlations, are predicted to hold in the classical counterpart (or infinite mass limit) of the model already for finite n on basis of the hydrodynamic approximation in spin-wave theory.[4] The proof of the large n result analogous to the one in the theorem for the classical n-vector spin model has been done in ref 5. The reason for the validity, in our quantum model, at any non-zero temperature, of the classical large distance asymptotics of the displacement correlations is made clear during the proof in Section 3.

4. A study of the fluctuations in the quantum model should include all observables, not just displacements. The techniques developed in ref. 1 are mainly suited for the latter, while the momenta require further consideration. Nontrivial quantum effects are known to be present for momentum fluctuations at a particular point of the phase diagram in another model of anharmonic crystal with the same Hartree–Fock approximation as the one we consider here.[6] A few remarks on the quantum character of the fluctuation algebra will be done in Section 5.

In Section 4 we consider the *global displacement fluctuation* $F_\delta(q)$ obtained from the local ones by summing over translations, as well, i.e., the limit in distribution as $N \to \infty$ of

$$F_\delta^{(N)}(q) = |\Lambda_N|^{-(1+\delta)/2} \sum_{x \in \Lambda_N} F^{(N)}(q_x) \tag{1.7}$$

(with δ chosen such as to get a nontrivial distribution of $F_\delta(q)$) and compare it with the Hartree–Fock approximation $\tilde{F}_{\tilde{\delta}}^{(N)}(q)$. The values of the critical exponents $\delta, \tilde{\delta}$ are both quite sensitive to the way of approaching an extremal state in the ferroelectric region, but typically $\delta < \tilde{\delta}$. In particular, for lattice dimension larger than 4, it is possible to have $\delta = 0$ (i.e., the "exact" fluctuations are *normal*), while the Hartree–Fock fluctuations (in extremal states) are always abnormally large in the multiphase region including the critical line. The fact that the Hartree–Fock approximation is more *singular* than the *n*-vector model is in correspondence with the standard wisdom that mean field approximations enhance phase transitions.

2. THE LOCAL DISPLACEMENT FLUCTUATION FIELD OF THE INFINITE CRYSTAL

In this section we give a short presentation of the model and a few results of ref. 1 in the translation invariant situation considered here, and perform the thermodynamic limit. In particular we describe the phase diagram and the construction of the local displacement fluctuation field.

2.1. The Model

The equilibrium positions of the oscillators are the sites of the cubic lattice $\mathbf{Z}^d$. The displacement of each oscillator from its equilibrium position $x \in \mathbf{Z}^d$ is a n-dimensional position operator $\vec{q}_x = (q_x^\alpha)_{\alpha=1,\dots,n} \in \mathbf{R}^n$ and the associated momenta are $p_x^\alpha = -i\partial/\partial q_x^\alpha$. We denote Λ_N the cube $\{x \in \mathbf{Z}^d;\ 0 \leqslant x_l < N,\ l = 1,\dots, d\}$ wrapped on a torus (periodic boundary conditions). The model Hamiltonian (where we restrict for definiteness to nearest neighbour harmonic interactions) is given by

$$H_{N,n} = \sum_{\alpha=1}^{n} \left\{ \sum_{x \in \Lambda_N} [(p_x^\alpha)^2/2m - hq_x^\alpha + (a/2)(q_x^\alpha)^2 + (b/2)(\vec{q}_x^{\,2}/n)^2] \right.$$
$$\left. + \frac{1}{2} \sum_{\substack{x,\, y \in \Lambda \\ |x-y|=1}} (q_x^\alpha - q_y^\alpha)^2 \right\} \tag{2.1}$$

The coupling-between different components comes only from the quartic term

$$(b/2n)(\vec{q}_x^{\,2})^2 = (b/2)\left((n^{-1/2})\sum_{\alpha=1}^{n}(q_x^\alpha)^2\right)^2$$

which for $b>0$ ensures the confinement. The quadratic one-site term $(a/2)\,\vec{q}_x^{\,2}$ may induce a ferroelectric phase transition if $a<0$. The external field $\vec{h}_x = (h)_{\alpha=1,\dots,n}$, violating the isotropy, is chosen along the main diagonal of $\mathbf{R}^n$, with the effect that the model has still full permutation invariance with respect to components α.

Let us denote by

$$f_{N,n} = \frac{-1}{n\beta\,|\Lambda_N|}\ln Z_{N,n}; \qquad Z_{N,n} = \operatorname{tr}\exp(-\beta H_{N,n}) \tag{2.2}$$

its free-energy per component,and per lattice site, and by

$$\langle\cdot\rangle_{N,n} = Z_{N,n}^{-1}\operatorname{tr}(\cdot\exp(-\beta H_{N,n})) \tag{2.3}$$

its finite-volume equilibrium state. In ref. 1 we derived, for every fixed N, the complete asymptotic series in powers of $1/n$ of $f_{N,n}$ and of $\langle O\rangle_{N,n}$ for any observable O depending on a finite number of components α. The leading term of these expansions are given by the Hartree–Fock approximation to the model (2.1), to be described below.

The Hartree–Fock approximation to Hamiltonian (2.1) is a self-consistent one, describing independent copies of scalar coupled harmonic oscillators, each system corresponding to one component and having the Hamiltonian

$$\begin{aligned}\tilde{H}_N(\mathbf{c}) = &\sum_{x\in\Lambda}\left[p_x^2/2m - hq_x + (a+2bc_x)\,q_x^2/2 - bc_x^2/2\right]\\ &+\sum_{\substack{x,\,y\in\Lambda\\|x-y|=1}}(q_x-q_y)^2/2\end{aligned} \tag{2.4}$$

where the numbers c_x, $x\in\Lambda_N$ are determined as solution of the self-consistency equation system: for all $x\in\Lambda_N$,

$$c_x = \langle q_x^2\rangle_{\tilde{\mathbf{c}},N} \tag{2.5}$$

where we denoted $\langle\cdot\rangle_{\tilde{\mathbf{c}},N}$ the equilibrium state at inverse temperature β of the Hamiltonian $\tilde{H}_N(\mathbf{c})$.

Translation invariance, combined with the uniqueness of the solution of the system (2.5), provides the major simplification that $c_x = c$ for all $x \in \Lambda_N$, where c is the solution of a single equation. For what follows, it is convenient to introduce the variable,

$$z = a + 2bc \geqslant 0 \tag{2.6}$$

and bring all translation invariant operators to diagonal form using the Fourier basis in $\mathbf{C}^{\Lambda_N}$:

$$(\mathbf{e}_k)_x = |\Lambda_N|^{-1/2} \exp(-ikx) \tag{2.7}$$

where

$$k \in \Lambda_N^* = \left\{ k : k_l = \frac{2\pi n_l}{N}, n_l = 0, \pm 1, \pm 2,..., \pm (N/2 - 1), N/2, l = 1,..., d \right\}$$

In particular, the matrix X_z of the quadratic form defining the potential function in Eq. (2.4):

$$(X_z)_{x,\, y} = (z + 4d)\, \delta_{x,\, y} - 2\delta_{|x-y|,\, 1} \tag{2.8}$$

has the eigenvectors $\mathbf{e}_k$ with corresponding eigenvalues

$$z + \omega(k), \qquad \text{where} \quad \omega(k) = 4 \sum_{i=1}^{d} \sin^2 \frac{k^i}{2} \tag{2.9}$$

Equation (2.5) writes as

$$\frac{z - a}{2b} = \left(\frac{h}{z}\right)^2 + \frac{1}{\beta\, |\Lambda_N|} \sum_{j \in \mathbf{Z}} \sum_{k \in \Lambda_N^*} [z + \omega(k) + (2\pi \sqrt{m}\, j/\beta)^2]^{-1} \tag{2.5$'$}$$

and has a unique solution $z_N(\beta, m, h) > 0$. This, in turn, allows, by going to normal modes in Eq. (2.4), to obtain the simple, well-known expressions for the free-energy $\tilde{f}_N(z)$ and equilibrium expectations $\langle \cdot \rangle_{z,\, N}^{\sim}$ associated with the harmonic Hamiltonian (2.4) for any $z > 0$.

With this notation, the Hartree–Fock free-energy and state are defined by

$$f_N^{HF} = \tilde{f}_N(z_N(\beta, m, h)) \qquad \text{and} \qquad \langle \cdot \rangle_N^{HF} = \prod_{\alpha=1}^{\infty} \langle \cdot \rangle_{z_N(\beta, m, h),\, N}^{\sim} \tag{2.10}$$

The results of ref. 1 imply, for all values of the parameters and for any observable O depending on a finite number of components, the convergence

$$\lim_{n\to\infty} f_{N,n} = f_N^{HF}; \qquad \lim_{n\to\infty} \langle O \rangle_{N,n} = \langle O \rangle_N^{HF} \tag{2.11}$$

and also that the fluctuations $\{F^{(N,n)}(q_x); x \in \Lambda_N\}$ and $\{F^{(N,n)}(q_x^2); x \in \Lambda_N\}$ defined cf. Eq. (1.1) converge in $\langle \cdot \rangle_{N,n}$-distribution to Gaussian vectors with covariance matrices $C_{x,y}^{(N)}$ and $D_{x,y}^{(N)}$, given by the r.h.s. of Eqs. (3.6) and (3.7) of ref. 1, respectively. In the next subsection we write down the matrices $C^{(N)}$, $D^{(N)}$ in their diagonal (Fourier basis) representation.

2.2. The Operator $R_z^{(N)}$ and the Covariance Matrix $C_z^{(N)}$

As a preliminary, we remind that the central object entering the formulae and proofs of ref. 1 was the linear operator $R_z^{(N)}$ acting in the space $\mathscr{H}_N = L_2([0,1]) \otimes \mathbf{C}^{\Lambda_N}$ (i.e., the space "extended" by adding a time variable):

$$R_z^{(N)} = \beta^{-1}\left(X_z + \left(i\frac{\sqrt{m}}{\beta}\frac{d}{dt}\right)^2\right)^{-1} \qquad (z>0) \tag{2.12}$$

where $i(d/dt)$ denotes the selfadjoint differential operator defined by periodic boundary conditions on $[0, 1]$. The eigenvalues of $i(d/dt)$ are $\lambda_q = 2\pi q$, $q \in \mathbf{Z}$, with corresponding eigenfunctions $\psi_q(t) = \exp(-2\pi i q t)$. Taking into account also Eqs. (2.7) and (2.9), one obtains that $R_z^{(N)}$ has the kernel

$$(R_z^{(N)})_{x,y}(s,t) = |\Lambda_N|^{-1} \sum_{\substack{k \in \Lambda_N^* \\ q \in \mathbf{Z}}} r_z(k,q) \exp[ik(y-x) + 2\pi i q(t-s)] \tag{2.13}$$

where

$$r_z(k,q) = \frac{1/\beta}{z + \omega(k) + (2\pi\sqrt{m}\, q/\beta)^2} \tag{2.14}$$

It is important to note that the function $r_z \colon \mathbf{B}^d \times \mathbf{Z} \to \mathbf{R}_+$ (where $\mathbf{B}^d = [-\pi, \pi)^d$ is the Brillouin zone wrapped on a torus) is independent of N (so, the only volume dependence in Eq. (2.13) comes from the summation range Λ_N^*) and is a real-analytic function on $\mathbf{B}^d$ (i.e., a periodic real-analytic function on $\mathbf{R}^d$). The (β, m)-dependence of r_z is omitted for notational convenience.

Remarks. 1. The operator $R_z^{(N)}$ appeared in ref. 1 in a natural way via the Feynmann–Kac formula involving an oscillator-bridge process: $R_z^{(N)}$ is the covariance operator of the latter. It might be helpful to give the quantum-mechanical meaning of $R_z^{(N)}$: if $0 \leqslant s \leqslant t \leqslant 1$,

$$(R_z^{(N)})_{x,\, y}\,(s, t) = \langle q_x(s); q_y(t)\rangle_{z,\, N}^{\sim} = (R_z^{(N)})_{y,\, x}\,(t, s)$$

where $q_x(t) = \exp(-\beta t \widetilde{H}_N(c))\, q_x \exp(\beta t \widetilde{H}_N(c))$ with $c = (z-a)/2$, and where $\langle A; B\rangle_{z,N}^{\sim} = \langle AB\rangle_{z,N}^{\sim} - \langle A\rangle_{z,N}^{\sim}\langle B\rangle_{z,N}^{\sim}$ are the truncated expectations in the state $\langle\cdot\rangle_{z,N}^{\sim}$.

2. By the definition of the Hartree–Fock state as the infinite product of states $\langle\cdot\rangle_{z,N}^{\sim}$ for $z = z_N(\beta, m, h)$, one can readily calculate

$$\langle \widetilde{F}^{(N,n)}(A)\, \widetilde{F}^{(N,n)}(B)\rangle_N^{HF} = \langle A; B\rangle_{z,N}^{\sim}$$

In particular, one gets the covariance matrix of the Gaussian vector $\{\widetilde{F}^{(N,n)}(q_x), x \in \Lambda_n\}$ as

$$\widetilde{C}_{x,\, y}^{(N)} := \langle \widetilde{F}^{(N,n)}(q_x)\, \widetilde{F}^{(N,n)}(q_y)\rangle_N^{HF} = (R_z^{(N)})_{x,\, y}\,(0, 0) \qquad (z = z_N(\beta, m, h)) \tag{2.15}$$

In order to express the finite-volume covariance $C^{(N)}$ we shall need

$$[(R_z^{(N)})_{x,\, y}\,(s, t)]^2 = |\Lambda_N|^{-1} \sum_{\substack{k \in \Lambda_N^* \\ q \in \mathbf{Z}}} \varphi_z^{(N)}(k, q) \exp[ik(y-x) + 2\pi i q(t-s)] \tag{2.16}$$

where $\varphi_z^{(N)}$ is the convolution $r_z * r_z$ over $\Lambda_N^* \times \mathbf{Z}$:

$$\varphi_z^{(N)}(k, q) = |\Lambda_N|^{-1} \sum_{\substack{k' \in \Lambda_N^* \\ q \in \mathbf{Z}}} r_z(k-k', q-q')\, r_z(k', q') \tag{2.17}$$

Then, the operator A defined in ref. 1, Eq. (2.28), which is essentially the "extension" to $\mathscr{H}_\Lambda$ of the q^2 Hartree–Fock covariance, writes as:

$$\begin{aligned}
&(A_z^{(N)})_{x,\, y}(s, t) \\
&\quad = 2\beta b \langle q_x^2(s); q_y^2(t)\rangle_{z,N}^{\sim} \\
&\quad = \frac{2\beta b}{|\Lambda_N|} \sum_{\substack{k \in \Lambda_N^* \\ q \in \mathbf{Z}}} \left[\left[\varphi_z^{(N)}(k, q) + 2\left(\frac{h}{z}\right)^2 r_z(k, q)\right] \exp[ik(y-x) + 2\pi i q(t-s)]\right]
\end{aligned} \tag{2.18}$$

Finally, we define the matrix $C_z^{(N)}$, given by Eq. (3.7) of ref. 1, by the Fourier representation:

$$(C_z^{(N)})_{x,y} = |\Lambda_N|^{-1} \sum_{k \in \Lambda_N^*} c_z^{(N)}(k) \exp ik(y-x) \tag{2.19}$$

with

$$\begin{aligned} c_z^{(N)}(k) &= \sum_{q \in \mathbf{Z}} \left[r_z(k,q) - \frac{4\beta b(h/z)^2\, r_z(k,q)^2}{1 + 2\beta b(\varphi_z^{(N)}(k,q) + (h/z)^2\, r_z(k,q))} \right] \\ &= \sum_{q \in \mathbf{Z}} \frac{1}{\beta} \frac{1 + 2\beta b \varphi_z^{(N)}(k,q)}{4b(h/z)^2 + (z + \omega(k) + (2\pi \sqrt{m}\, q/\beta)^2)(1 + 2\beta b \varphi_z^{(N)}(k,q))} \end{aligned} \tag{2.20}$$

The covariance matrix $C^{(N)}$ of the local displacement fluctuations $F^{(N)}(q_x)$ is obtained by putting $z = z_N(\beta, m, h)$ in $C_z^{(N)}$.

Remarks. 1. We consider here the $N \to \infty$ limit of the expressions above for *fixed* $z > 0$. The general rule is that the Fourier sums converge to integrals. For instance,

$$\begin{aligned} \lim_{N \to \infty} (R_z^{(N)})_{x,y}(s,t) &= (R_z)_{x,y}(s,t) \\ &= (2\pi)^{-d} \int_{\mathbf{B}^d} dk \sum_{q \in \mathbf{Z}} r_z(k,q) \exp[ik(y-x) + 2\pi i q(t-s)] \end{aligned} \tag{2.21}$$

and also

$$\begin{aligned} \lim_{N \to \infty} \varphi_z^{(N)}(k,q) &= \varphi_z(k,q) \\ &= \sum_{q' \in \mathbf{Z}} (2\pi)^{-d} \int_{\mathbf{B}^d} dk'\, r_z(k-k', q-q')\, r_z(k', q') \end{aligned} \tag{2.22}$$

Applying the dominated convergence theorem in Eqs. (2.18), (2.19), one obtains that, uniformly on compacts of $z > 0$, all matrix elements $(A_z^{(N)})_{x,y}$ and $(C_z^{(N)})_{x,y}$ converge as $N \to \infty$ and the limit matrices A_z and C_z define bounded operators in $\boldsymbol{l}^2(\mathbf{Z}^d)$.

2. We conclude with a remark about the limit of $R_z^{(N)}$ in the case $z = 0$. If $d \geqslant 3$, the following limits exist and are finite:

$$\lim_{z \searrow 0} (R_z)_{x,y}(s,t) =: (R_0)_{x,y}(s,t)$$

Of course, for finite N, $\lim_{z\searrow 0} R_z^{(N)}$ does not exist because of the $k=0$, $q=0$ term; however, by projecting out the one-dimensional subspace of constant functions corresponding to it, i.e., by excluding $(k, q)=(0, 0)$ from the sum in Eq. (2.2), one defines a kernel $(R_z'^{(N)})_{x,y}$ for which the convergence (2.9) holds with $z=0$ included:

$$\lim_{N\to\infty} (R_z'^{(N)})_{x,y}(s,t)=(R_z)_{x,y}(s,t), \qquad \forall z \geqslant 0$$

Also, estimates on the rate of convergence in the last equation are known:[8] the error is exponentially small if $z>0$ (in view of the analyticity of the integrand) and it is $O(N^{2-d})$ if $z=0$ (in view of the singularity $\sim |k|^{-2}$ at $k=0$ of $r_z(k, 0)$).

2.3. The Phase Diagram

As already mentioned before, the thermodynamics of the model is given exactly by the Hartree–Fock approximation, therefore the phase diagram of the model is the same as the one obtained in ref. 6. We rederive briefly the result for further reference.

The parameters of the model are $\beta>0$, $m>0$ and h. The selfconsistency equation (2.5′) which we write again for convenience:

$$\frac{z-a}{2b}=\left(\frac{h}{z}\right)^2+(R_z^{(N)})_{x,x}(0,0) \tag{2.23}$$

has a unique solution $z_N(\beta, m, h)>0$, because the r.h.s. is strictly decreasing of z and diverges to $+\infty$ for $z\searrow 0$. The different regions of the phase diagram are determined by the $N\to\infty$ behaviour of $z_N(\beta, m, h)$. We henceforth suppose $a<0$ in order to have a nontrivial phase diagram.

If $h\neq 0$, the limit equation

$$\frac{z-a}{2b}=\left(\frac{h}{z}\right)^2+(R_z)_{x,x}(0,0) \tag{2.24}$$

has likewise a unique solution $z_\infty(\beta, m, h)>0$, and

$$\lim_{N\to\infty} z_N(\beta, m, h)=z_\infty(\beta, m, h) \tag{2.25}$$

If $h=0$, the limit equation

$$\frac{z-a}{2b}=(R_z)_{x,x}(0,0) \tag{2.24′}$$

has a positive solution $z_\infty(\beta, m, 0)$ if, and only if, $(R_0)_{x,x}(0,0) > -a/2b$ and, in this case, again Eq. (2.25) holds. Moreover, $z_\infty(\beta, m, h)$ is a real-analytic function in the whole (β, m, h)-region where it is strictly positive.

It is convenient to introduce a special notation for $(R_z)_{x,x}(0,0)$, putting into evidence its dependence on d, β and m:

$$\begin{aligned} I_d(\beta, m; z) &= (2\pi)^{-d} \int_{\mathbf{B}^d} dk \sum_{q \in \mathbf{Z}} r_z(k, q) \\ &= (2\pi)^{-d} \int_{\mathbf{B}^d} dk \frac{\coth(\beta/2\sqrt{m})\sqrt{z+\omega(k)}}{2\sqrt{m}\sqrt{z+\omega(k)}} \end{aligned} \tag{2.26}$$

This is a decreasing function of β and

$$I_d(\infty, m; z) = \frac{1}{2\sqrt{m}} (2\pi)^{-d} \int_{\mathbf{B}^d} dk \frac{1}{\sqrt{z+\omega(k)}}, \qquad (z > 0) \tag{2.27}$$

$I_d(\beta, m; 0+)$ is finite for $d \geqslant 2$. (Remark however that $I_2(\beta, m; z)$ behaves for $\beta \to \infty$, $z \to 0$ as $I_2(\infty, m; 0+) + \text{const}(|\ln z|/\beta)$, due to the $q = 0$ term in the sum (2.26)).

For $d \geqslant 3$, define m_d^* by

$$\frac{-a}{2b} = I_d(\infty, m_d^*; 0+), \qquad \text{i.e.,} \quad m_d^* = \left(\frac{b}{a} (2\pi)^{-d} \int_{\mathbf{B}^d} dk \frac{1}{\sqrt{\omega(k)}}\right)^2 \tag{2.28}$$

and $\beta_c(m)$ for $m > m_d^*$ by

$$\frac{-a}{2b} = I_d(\beta_c(m), m; 0+) \tag{2.29}$$

With these definitions one can describe the phase diagram of the model in the following form:

In the region

$$D_1 = \{h \neq 0\} \cup \{h = 0, m < m_d^*, \beta < \beta_c(m)\}$$

one has one normal phase, depending analytically on β, m, h. For $(\beta, m, h) \in D_1$, $\lim_{N \to \infty} z_N(\beta, m, h) = z_\infty(\beta, m, h) > 0$ and all quantities of interest are obtained by applying the rule $|\Lambda_N|^{-1} \sum_{k \in \Lambda_N^*} \to (2\pi)^{-d} \int_{\mathbf{B}^d} dk$, e.g., using the short-hand notation lim for the iterated limit $\lim_{N \to \infty} \lim_{n \to \infty}$ and z for $z_\infty(\beta, m, h)$, one gets in the limit for the displacement average and Hartree–Fock covariance:

$$\lim \langle q_x^\alpha \rangle_{N,n} = \frac{h}{z} =: M(\beta, m, h) \tag{2.30}$$

$$\begin{aligned}\lim \langle q_x^\alpha; q_y^\alpha \rangle_{N,n} &= (R_z)_{x,y}(0,0) \\ &= (2\pi)^{-d} \int_{\mathbf{B}^d} \frac{\coth(\beta/2\sqrt{m})\sqrt{z+\omega(k)}}{2\sqrt{m}\sqrt{z+\omega(k)}} \exp ik(y-x)\, dk \\ &=: (\tilde{C}_z)_{x,y}\end{aligned} \tag{2.31}$$

Remark. The existence of a critical mass $m_d^* > 0$ below which there is no long-range order in the whole temperature range is a manifestation of a general phenomenon, first evidentiated in ref. 9, namely that strong quantum fluctuations prevent the appearance of the ordered phase. A suppression of corresponding abnormal fluctuations was proven later in ref. 10.

In the region

$$D_2 = \{h = 0, m > m_d^*, \beta > \beta_c(m)\}$$

one has multiple phases. One can select an extremal state by approaching a point (β, m) in D_2 by points in D_1 and looking at the weak limit of the unique infinite-volume states associated to the latter, e.g., by letting $h \searrow 0$ in Eqs. (2.30)–(2.31). One has $\lim_{h \searrow 0} z_\infty(\beta, m, h) = 0$ and the state has spontaneous displacement:

$$M(\beta, m) = \frac{-a}{2b} - I_d(\beta, m; 0+) > 0 \tag{2.32}$$

and the Hartree–Fock covariance operator

$$(\tilde{C}_0)_{x,y} = (2\pi)^{-d} \int_{\mathbf{B}^d} \frac{\coth(\beta\sqrt{\omega(k)}/2\sqrt{m})}{2\sqrt{m}\sqrt{\omega(k)}} \exp ik(y-x)\, dk \tag{2.33}$$

has power law decay as $|x-y| \to \infty$.

Remark. Another way of selecting the extremal state is to look at limits of finite volume states $\langle \cdot \rangle_N^{HF}$ in a volume-dependent external field h_N such that $\lim_N (h_N / z_N(\beta, m, h_N)) = M(\beta, m)$, e.g., $h_N \sim |\Lambda_N|^{-\alpha}$ with $0 < \alpha < 1$ ($\alpha < 1$ ensures that $z_N |\Lambda_N| \to \infty$, therefore all sums in the second term of the self-consistency Eq. (2.5′) converge to integrals, yielding $I_d(\beta, m; 0+)$), cf. refs. 6 and 7. While the state and the local fluctuation field obtained by the two procedures are the same, the global fluctuations turn out to be quite sensitive to the fine tuning of the external field, see Section 4.

Finally, the line

$$D_3 = \{h=0,\, m > m_d^*,\, \beta = \beta_c(m)\}$$

is a line of critical points, with no spontaneous displacement $M(\beta_c(m), m) = 0$, and Hartree–Fock covariance given by Eq. (2.33).

2.4. The Local-Displacement Fluctuation Field

In the regularity region D_1 of the phase diagram, where $\lim_N z_N = z_\infty > 0$ (the dependence on $(\beta, m, h) \in D_1$ is understood), one has from Eq. (2.22) that

$$\lim_{N\to\infty} \varphi^{(N)}_{z_N}(k, q) = \varphi_{z_\infty}(k, q) \tag{2.34}$$

The convergence is uniform on $\mathbf{B}^d$ and the functions $\varphi_{z_\infty}(\cdot, q)$ are real-analytic for all $q \in \mathbf{Z}$. One obtains therefore that

$$\lim_{N\to\infty} (C^{(N)}_{z_N})_{x,y} = (C_{z_\infty})_{x,y} = (2\pi)^{-d} \int_{\mathbf{B}^d} c_{z_\infty}(k) \exp ik(y-x)\, dk \tag{2.35}$$

where $c_z \colon \mathbf{B}^d \to \mathbf{R}$ $(z > 0)$ is the real analytic function

$$c_z(k) = \sum_{q\in\mathbf{Z}} \frac{1}{\beta} \frac{1 + 2\beta b \varphi_z(k, q)}{4b(h/z)^2 + (z + \omega(k) + (2\pi \sqrt{m}\, q/\beta)^2)(1 + 2\beta b \varphi_z(k, q))} \tag{2.36}$$

Hence, $(C_{z_\infty})_{x,y}$ decays exponentially fast as $|x-y| \to \infty$ and therefore the matrix C_{z_∞} defines a bounded operator on $\mathbf{l}_2(\mathbf{Z}^d)$. Summarizing, we have the following

Lemma. (i) For $(\beta, m, h) \in D_1$ the finite-dimensional distributions of the finite-volume displacement fluctuation vectors $F^{(N)}(q_x)$, $x \in \Lambda_N$ converge to the finite-dimensional distributions of a regular Gaussian field $F(q_x)$, $x \in \mathbf{Z}^d$, of covariance operator C_{z_∞}. The same picture holds for the Hartree–Fock fluctuations $\tilde{F}^{(N)}(q_x)$, which converge in finite distribution to another regular Gaussian field $\tilde{F}(q_x)$, $x \in \mathbf{Z}^d$ of covariance operator $\tilde{C}_{z_\infty}$ defined by the matrix (2.31).

(ii) For (β, m) in the multiphase region D_2 and on the critical line D_3 we define the fluctuation field by taking the limit in finite distributions as $h \searrow 0$ of the regular field corresponding to $(\beta, m, h) \in D_1$. The limit is a singular Gaussian field of covariance matrix

$$(C_0)_{x,y} = \lim_{z \searrow 0} (C_z)_{x,y} = (2\pi)^{-d} \int_{\mathbf{B}^d} c_0(k) \exp ik(y-x)\, dk \tag{2.37}$$

with

$$c_0(k) = \sum_{q \in \mathbf{Z}} \frac{1}{\beta} \frac{1 + 2\beta b \varphi_0(k, q)}{4b\tilde{m}(\beta, m)^2 + (\omega(k) + (2\pi \sqrt{m}\, q/\beta)^2)(1 + 2\beta b \varphi_0(k, q))} \tag{2.38}$$

where

$$\varphi_0(k, q) = \sum_{q' \in \mathbf{Z}} (2\pi)^{-d} \int_{\mathbf{R}^d} dk'\, r_0(k-k', q-q')\, r_0(k', q') \tag{2.39}$$

Likewise, the same limit of $\{\tilde{F}(q_x); x \in \mathbf{Z}^d\}$ defines a singular Gaussian field of covariance matrix $\tilde{C}_0$, Eq. (2.33).

In order to facilitate the comparison with the Hartree–Fock covariance, we use in Eq. (2.33) the well-known identity

$$\tilde{c}_0(k) := \frac{\coth(\beta \sqrt{\omega(k)}/2 \sqrt{m})}{2 \sqrt{m} \sqrt{\omega(k)}} = \sum_{q \in \mathbf{Z}} \frac{1}{\beta} \frac{1}{\omega(k) + (2\pi \sqrt{m}\, q/\beta)^2} \tag{2.40}$$

3. CLUSTERING PROPERTIES OF THE LOCAL FLUCTUATION FIELD

In this section we prove the theorem in the Introduction, i.e., we establish and compare the large distance decay properties of $(C_0)_{x,y}$ defined in Eqs. (2.37)–(2.38) and of the Hartree–Fock covariance $(\tilde{C}_0)_{x,y}$, Eq. (2.33). These relations will be proved in the following weak (distribution) sense:

Definition. A function $f: \mathbf{Z}^d \to \mathbf{R}$ is said to have the weak limit $L \in \mathbf{R}$ as $x \to \infty$ if, for every C^∞ function $\Phi: \mathbf{R}^d \to \mathbf{R}$ with compact support away from the origin

$$\lim_{\lambda \to \infty} \lambda^{-d} \sum_{x \in \mathbf{Z}^d} f(x)\, \Phi(x/\lambda) = L \int_{\mathbf{R}^d} \Phi(x)\, dx = L(2\pi)^{d/2}\, \hat{\Phi}(0) \tag{3.1}$$

The meaning of this definition is that the measure defined by point masses equal to $f(x)$ placed at the point $x/\lambda \in (1/\lambda)\, \mathbf{Z}^d$ (i.e., the contracted cubic lattice of lattice constant $1/\lambda$) converges weakly to $L\,dx$ outside the origin. Clearly, usual convergence to the limit L implies weak convergence to L, so, if the limit exists, it equals the weak limit. The converse is not true (e.g., take $f(x)=(-1)^{\sum_{i=1}^{d} x_i}$ for which the weak limit exists and equals 0 but the usual limit does not exist) because Eq. (3.1) implies an averaging process over a large scale.

Lemma. The following large distance asymptotics hold weakly:

$$\lim_{|x-y|\to\infty} |x-y|^{d-2}\,(\tilde{C}_0)_{x,y} = \frac{1}{\beta} K_d, \qquad \text{if} \quad (\beta, m) \in D_2 \cup D_3 \tag{3.2}$$

$$\lim_{|x-y|\to\infty} |x-y|^{2(d-2)}\,(C_0)_{x,y} = \frac{1}{2\beta M^2} K_d^2, \qquad \text{if} \quad (\beta, m) \in D_2 \tag{3.3}$$

$$\lim_{|x-y|\to\infty} |x-y|^{d-2}\,(C_0)_{x,y} = \frac{1}{\beta} K_d, \qquad \text{if} \quad (\beta, m) \in D_3 \tag{3.4}$$

where $K_d = \Gamma(d/2-1)/4\pi^{d/2}$.

Remarks. 1. For $(\beta, m)\in D_3$, i.e., where $M(\beta, m)=0$, $(C_0)_{x,y} = (\tilde{C}_0)_{x,y}$, as seen by comparing Eqs. (2.38) and (2.40). Hence, Eq. (3.4) coincides with Eq. (3.2).

2. The most significant result is Eq. (3.3), which proves the theorem in the Introduction, i.e., shows that, whenever $M(\beta, m)>0$, $(C_0)_{x,y}$ behaves at large distances like $(\tilde{C}_0)^2_{x,y}$. For instance, if $d=3$, $(\tilde{C}_0)_{x,y} \sim (1/\beta)\,|x-y|^{-1}$, while $(C_0)_{x,y} \sim (1/2\beta M^2)\,|x-y|^{-2}$ (with an amplitude diverging as the critical line is approached).

3. While $\sum_{y\in\mathbf{Z}^d} (\tilde{C}_0)_{x,y}$ diverges for all $d\geqslant 3$, one has $\sum_{y\in\mathbf{Z}^d} (C_0)_{x,y}$ convergent for $d\geqslant 5$ and divergent only for $d=3, 4$. In particular, defining the global fluctuations in the infinite-volume state as the limit in distribution as $N\to\infty$ of

$$F_{N,\delta} = |\Lambda_N|^{-(1+\delta)/2} \sum_{x\in\Lambda_N} F(q_x), \qquad \tilde{F}_{x,\tilde{\delta}} = |\Lambda_N|^{-(1+\tilde{\delta})/2} \sum_{x\in\Lambda_N} \tilde{F}(q_x) \tag{3.5}$$

then, in order to get nontrivial limit random variables, one should take $\delta = \delta(d)$, $\tilde{\delta} = \tilde{\delta}(d)$ as follows:

$$\tilde{\delta}(d) = \frac{1}{d}, \forall d \geqslant 3, \qquad \delta(d) = \begin{cases} 1/6, & \text{if} \quad d = 3 \\ 0+, & \text{if} \quad d = 4 \\ 0, & \text{if} \quad d \geqslant 5 \end{cases} \tag{3.6}$$

(where $0+$ means modulo logarithmic corrections). This means that the global fluctuations associated in an extremal infinite-volume state with $F(q_x)$ become normal starting with $d = 4$, where, in fact, the mean-field behaviour is expected to set in.

4. The same relations (3.2)–(3.4) hold for the classical counterpart of the model (or its infinite mass limit $m \to \infty$). This follows from the fact that the Fourier coefficients of a real analytic function on $\mathbf{B}^d$ have exponential decay. As $\omega(k)$, and hence $(a + \omega(k))^{-1}$ for $a > 0$, is real analytic and as the series (2.38) and (2.40) are uniformly convergent, one concludes that only the $q = 0$ terms contribute to the power law asymptotics. In particular, $\tilde{c}_0(k)$ can be replaced by $1/\beta\omega(k)$ (which is its classical counterpart), and hence Eq. (3.2) is nothing but the well known asymptotic behaviour of the kernel of $(-\varDelta)^{-1}$, where $\varDelta$ is the lattice Laplacian. By the same argument $\varphi_0(k, q)$ equals, modulo a real analytic function on $\mathbf{B}^d$, the $q' = 0$ term in its definition (2.39), i.e., its classical counterpart:

$$\varphi_0(k, q) \sim (2\pi)^{-d} \int_{\mathbf{B}^d} dk' \, \frac{1}{\omega(k - k') \, \omega(k')} =: \varphi_0^{\text{sing}}(k, q) \tag{3.7}$$

where $\sim$ means equality of the singular parts. As it will become clear during the proof, neither the latter replacements affect the power-law decay.

Proof of Eq. (3.3). We take $f(x) = |x|^{2(d-2)} \, (C_0)_{0,x}$ in the definition above and use the fact that the function $|x|^{2(d-2)} \, \varPhi(x)$ is likewise C^∞ with compact support outside the origin, therefore its Fourier transform, which equals $(-\varDelta)^{d-2} \, \hat{\varPhi}(k)$, has all moments equal to 0. Therefore,

$$\lambda^{-d} \sum_{x \in \mathbf{Z}^d} |x|^{2(d-2)} \, (C_0)_{0,x} \, \varPhi(x/\lambda) = \lambda^{d-4} \int_{\mathbf{R}^d} c_0(k/\lambda)(-\varDelta)^{d-2} \, \hat{\varPhi}(k) \, dk \tag{3.8}$$

will not charge if we modify c_0 by subtracting an arbitrary polynomial of k (the convergence at infinity is ensued by the fact that $\hat{\varPhi} \in \mathscr{S}(\mathbf{R}^d)$, i.e., it decays at ∞, with all its derivatives, faster than any inverse power of distance). This is the main technical advantage of the definition (3.1): we are no longer bound to work with equivalence modulo real analytic *periodic* functions.

Summarizing, in order to obtain Eq. (3.3), we have to show that

$$\lim_{\lambda\to\infty} \lambda^{d-4} \int_{\mathbf{R}^d} c_0(k/\lambda)(-\Delta)^{d-2}\, \hat{\Phi}(k)\, dk = \frac{K_d^2}{2\beta M^2} \int_{\mathbf{R}^d} \psi_d(k)(-\Delta)^{d-2}\, \hat{\Phi}(k)\, dk \tag{3.9}$$

where $\psi_d(k)$ is the fundamental solution of $(-\Delta)^{d-2}\, \psi_d(k) = \delta$:[11]

$$\psi_d(k) = \begin{cases} A_d\, |k|^{d-4} & (d \text{ odd}) \\ B_d\, |k|^{d-4} \ln |k| & (d \text{ even}) \end{cases} \tag{3.10}$$

Thereby, we can subtract at will polynomials from c_0, meaning that only the singular part of c_0 will contribute to the limit (3.9). We shall denote $\approx$ the equality modulo a polynomial.

Applying this machinery to Eq. (3.9) one has successively

$$\begin{aligned}
\lambda^{d-4} c_0(k/\lambda) &\approx \frac{\lambda^{d-4}}{\beta} \frac{1+2\beta b \varphi_0(k/\lambda, 0)}{4bM^2 + \omega(k/\lambda)(1+2\beta b\varphi_0(k/\lambda, 0))} \\
&= \frac{\lambda^{d-4}}{4b\beta M^2} \sum_{p=0}^{s-1} (-1)^p \left(\frac{\omega(k/\lambda)}{4bM^2}\right)^p (1+2\beta\varphi_0(k/\lambda, 0))^{p+1} \\
&\quad + \frac{(-1)^s\, \lambda^{d-4} (\omega(k/\lambda)/4bM^2)^s\, (1+2\beta b\varphi_0(k/\lambda, 0))^{s+1}}{\beta(4bM^2 + \omega(k/\lambda)(1+2\beta b\varphi_0(k/\lambda, 0)))} \\
&\approx \frac{\lambda^{d-4} \varphi_0^{\text{sing}}(k/\lambda, 0)}{2\beta M^2} \\
&\quad + \frac{\lambda^{d-4}}{4b\beta M^2} \sum_{p=1}^{s-1} (-1)^p \left(\frac{\omega(k/\lambda)}{4bM^2}\right)^p (1+2\beta b\varphi_0(k/\lambda, 0))^{p+1} \\
&\quad + \frac{(-1)^s\, \lambda^{d-4} (\omega(k/\lambda)/4bM^2)^s\, (1+2\beta b\varphi_0(k/\lambda, 0))^{s+1}}{\beta(4bM^2 + \omega(k/\lambda)(1+2\beta b\varphi_0(k/\lambda, 0)))}
\end{aligned} \tag{3.11}$$

At this stage it should be visible that the first term alone provides the stated result: indeed, φ_0^{sing} is the convolution $1/\omega * 1/\omega$, so its Fourier transform behaves like the square of the Fourier transform of $1/\omega$. In fact, φ_0^{sing} has been analyzed in connection with the classical n-vector model in ref. 5, where it is proved that there exist functions $R_\lambda(k)$ such that

$$\varphi_0^{\text{sing}} \approx R_\lambda \qquad \text{and} \qquad \lim_{\lambda\to\infty} \lambda^{d-4} R_\lambda(k/\lambda) = (2\pi)^d\, K_d^2 \psi_d(k) \tag{3.12}$$

We are thus left with showing that the other terms in Eq. (3.11) converge to zero as $\lambda \to \infty$. We shall use that for $k \in \mathbf{B}^d$

$$C' \, |k|^2 \leqslant \omega(k) \leqslant C \, |k|^2, \qquad \lim_{\lambda \to \infty} \lambda^2 \omega(k/\lambda) = |k|^2 \tag{3.13}$$

$$0 \leqslant \varphi_0(k, 0) \leqslant \begin{cases} C/|k|, & \text{if} \quad d = 3 \\ C \, |\ln |k||, & \text{if} \quad d = 4 \\ C & \text{if} \quad d \geqslant 5 \end{cases} \tag{3.14}$$

One can see from these bounds, by simple power counting and applying the dominated convergence theorem, that the last term of Eq. (3.11) does not contribute to the limit (3.9), if the following choice of s is done: $s = 1$ for $d = 3, 4$ and $s = [d/2] - 1$ for $d \geqslant 5$ (Indeed, this term is $O(\lambda^{-1})$ for $d = 3$, $O(|k|^2 \ln^2 \lambda/\lambda^2 \, |\ln |k||)$ for $d = 4$, and $O(|k|^{2s} \lambda^{d-4-2s})$ for $d \geqslant 5$). We have still to settle the middle terms $p = 1,..., s-1$ for $d > 5$. Using Eq. (3.12) one sees that the singular part is given by terms of the form

$$\lambda^{d-4} \omega(k/\lambda)^p \, R_\lambda(k/\lambda)^n \, P_m(k/\lambda)$$

where P_m is a homogeneous polynomial of degree $m \geqslant 0$ and $1 \leqslant n \leqslant p+1$. Therefore, using Eqs. (3.12), (3.13) and (3.14), one has that the contribution of this term is bounded by

$$\lambda^{d-4-2p-m-n(d-4)} (\lambda^2 \omega(k/\lambda))^p \, |\lambda^{d-4} R_\lambda(k/\lambda)|^n$$

which vanishes when $\lambda \to \infty$. ∎

4. GLOBAL DISPLACEMENT FLUCTUATIONS

We shall calculate here the critical exponents δ of the global displacement fluctuations $F_\delta^{(N)}(q)$, Eq. (1.7), in the multiphase region D_2, where differences from the Hartree–Fock value $\tilde{\delta}$ may appear. When considering the infinite-volume limit of $F_\delta^{(N)}(q)$ and $\tilde{F}_{\tilde{\delta}}^{(N)}(q)$ with respect to the finite-volume equilibrium distributions, one has to make sure, in order to obtain a significant result (i.e., $\delta < 1/2$), that the latter approach an extremal infinite-volume state. We shall do this via the procedure described in the remark of Section 2.3, i.e., by taking finite-volume states with an external field h_N, vanishing as $N \to \infty$. Namely, we take

$$h_N = |\Lambda_N|^{-\alpha}, \qquad 0 < \alpha < 1 \tag{4.1}$$

and look at $F_{\delta}^{(N)}(q)$ and $\tilde{F}_{\tilde{\delta}}^{(N)}(q)$ constructed as in Eq. (1.7) in terms of the Gaussian vectors $F_{\delta}^{(N)}(q_x)$ and $\tilde{F}_{\tilde{\delta}}^{(N)}(q_x)$, $x \in \Lambda_N$, of covariance matrices $C^{(N)} = C_{z_N(\beta, m, h_N)}^{(N)}$ (Eq. (2.19), (2.20)) and $\tilde{C}^{(N)} = R_{z_N(\beta, m, h_N)}^{(N)}(0, 0)$ (Eq. (2.15)), respectively. The condition of extremality of the limit state is expressed as:

$$\lim_{N \to \infty} \frac{h_N}{z_N(\beta, m, h_N)} = M(\beta, m) \tag{4.2}$$

i.e., $z_N \sim M(\beta, m)^{-1} |\Lambda_N|^{-\alpha}$. Remembering Eq. (2.32), this implies that the term $j=0, k=0$ of the self-consistency Eq. (2.5′) should go to 0, i.e., that $z_N |\Lambda_N| \to \infty$, which requires $\alpha < 1$.

As a result, $F_{\delta}^{(N)}(q)$ and $\tilde{F}_{\tilde{\delta}}^{(N)}(q)$ are Gaussian random variables of variances, respectively:

$$c_{z_N}^{(N)}(0) = \frac{1}{\beta |\Lambda_N|^{2\delta}} \sum_{q \in \mathbf{Z}} \frac{1 + 2\beta b \varphi_{z_N}^{(N)}(0, q)}{4b(h_N/z_N)^2 + (z_N + (2\pi \sqrt{m}\, q/\beta)^2)(1 + 2\beta b \varphi_{z_N}^{(N)}(0, q))} \tag{4.3}$$

$$\tilde{c}_{z_N}^{(N)}(0) = \frac{1}{\beta |\Lambda_n|^{2\tilde{\delta}}} \sum_{q \in \mathbf{Z}} \frac{1}{(z_N + (2\pi \sqrt{m}\, q/\beta)^2)} \tag{4.4}$$

Thereby, $\delta = \delta(\alpha)$ and $\tilde{\delta} = \tilde{\delta}(\alpha)$ are to be chosen such that the limits of (4.3) and (4.4), respectively, be different from 0 and ∞. It is obvious from Eq. (4.2) that, for all $d \geqslant 3$ and all $(\beta, m) \in D_2$,

$$\tilde{\delta}(\alpha) = \alpha/2 \tag{4.5}$$

which is exactly the result obtained in ref. 6.

In order to calculate $\delta(\alpha)$, we need the asymptotics of

$$\begin{aligned} \varphi_{z_N}^{(N)}(0, 0) &= \frac{1}{|\Lambda_N|} \sum_{k, q} [z_N + \omega(k) + (2\pi \sqrt{m}\, q/\beta)^2]^{-2} \\ &\sim \frac{1}{|\Lambda_N|} \sum_{k} [z_N + \omega(k)]^{-2} \end{aligned} \tag{4.6}$$

Let $d = 3$. If $\alpha > 2/3$, taking into account that the sum in Eq. (4.6) is over $k = 2\pi |\Lambda_N|^{-1/3} \kappa$, $\kappa \in \mathbf{Z}^3$ and using the bound (3.13), one has:

$$\begin{aligned} z_N + \omega(k) &\sim M^{-1} |\Lambda_N|^{-\alpha} + \omega(2\pi |\Lambda_N|^{-1/3} \kappa) \\ &\geqslant M^{-1} |\Lambda_N|^{-\alpha} + C |\Lambda_N|^{-2/3} \kappa^2 \end{aligned}$$

hence

$$|\Lambda_N|^{-1} \sum_{k \neq 0} [z_N + \omega(k)]^{-2} \leqslant |\Lambda_N|^{1/3} \sum_{\kappa \in \mathbf{Z}^3 \setminus \{0\}} \kappa^{-2}$$

therefore the $k = 0$ term $|\Lambda_N|^{-1} z_N^{-2} \sim M^2 |\Lambda_N|^{2\alpha - 1}$ dominates the $N \to \infty$ behavior. On the other hand, if $\alpha < 2/3$, $|\Lambda_N|^{-1} z_N^{-3/2} \to 0$, and using the convergence of the integral

$$J = \int_{\mathbf{R}^3} (1 + k^2)^{-1} \, dk$$

together with the limit in Eq. (3.13), one has

$$\begin{aligned} \varphi_{z_N}^{(N)}(0, 0) &\sim |\Lambda_N|^{-1} z_N^{-2} \sum_{k \in \Lambda_N^*} [1 + z_N^{-1} \omega(k)]^{-2} \\ &= z_N^{-1/2} (|\Lambda_N|^{-1} z_N^{-3/2}) \sum_{k \in z_N^{-1/2} \Lambda_N^*} [1 + z_N^{-1} \omega(z_N^{1/2} k)]^{-2} \sim z_N^{-1/2} J \end{aligned}$$

Returning to Eq. (4.3), and remarking that in all cases $z_N \varphi_{z_N}^{(N)}(0, 0) \to 0$, one obtains

$$\delta(\alpha) = \begin{cases} \alpha/4, & \alpha \leqslant 2/3 \\ \alpha - 1/2, & \alpha > 2/3 \end{cases} \qquad (d = 3) \tag{4.7}$$

Let now $d = 4$. Using again the bounds (3.13), one has

$$\varphi_{z_N}^{(N)}(0, 0) \sim |\Lambda_N|^{-1} z_N^{-2} + \sum_{\substack{\kappa \in \mathbf{Z}^4 \setminus \{0\} \\ |\kappa_i| \leqslant N}} (|\Lambda_N|^{-\alpha + 1/2} + C\kappa^2)^{-2}$$

if $\alpha > 1/2$, the first term, being proportional to $|\Lambda_N|^{2\alpha - 1}$, dominates the second term proportional to $\ln |\Lambda_N|$, while, if $\alpha < 1/2$, the converse is true. One obtains therefore

$$\delta(\alpha) = \begin{cases} 0+, & \alpha \leqslant 1/2 \\ \alpha - 1/2, & \alpha > 1/2 \end{cases} \qquad (d = 4) \tag{4.8}$$

Finally, let $d \geqslant 5$. Then $J_d := \int_{\mathbf{B}^d} \omega(k)^2 \, dk < \infty$, therefore

$$\lim_{N \to \infty} (\varphi_{z_N}^{(N)}(0,0) - |\Lambda_N|^{-1} z_N^{-2}) = (2\pi)^{-d} J_d$$

and one gets

$$\delta(\alpha) = \begin{cases} 0, & \alpha \leqslant 1/2 \\ \alpha - 1/2, & \alpha > 1/2 \end{cases} \qquad (d \geqslant 5) \tag{4.9}$$

We remark that the Hartree–Fock values $\tilde{\delta}(\alpha)$ in Eq. (4.5) are strictly larger than $\delta(\alpha)$ for all $\alpha \neq 0, 1$. The difference $\tilde{\delta}(\alpha) - \delta(\alpha) > 0$ expresses quantitatively the fact that, even in the $n \to \infty$ limit, the n-component vector model takes into account *more correlations* than the Hartree–Fock model, yielding a better approximation of the finite-component model. Remark also that $\lim_{\alpha \searrow 0} \delta(\alpha) = 0$, expressing the normality of the fluctuations if the external field tends to zero slowly enough such that it induces a quadratic deviation from the equilibrium free-energy. For $\alpha \geqslant 1$, $\tilde{\delta}(1) = \delta(1) = 1/2$, characteristic for phase mixtures, indicating that the external field is too weak to pick up an extremal state. Anyway, these results show that the abnormal character of the fluctuations is sensitive to boundary conditions, in particular to external fields.

5. REMARKS

The $1/n$-expansion[1] allows to construct for the n-vector anharmonic crystal an interacting field of local-displacement fluctuations $\{F^{(N)}(q_x)\}_{x \in \Lambda_N}$ in the limit $n = \infty$.

We have studied the clustering properties of this field in the thermodynamic limit for different domains of the phase diagram and compared them with the corresponding Hartree–Fock approximation. The latter yields for $\tilde{F}(q_x)$, $x \in \mathbf{Z}^d$, the same results as for the exactly soluble spherical model for a one-component anharmonic crystal.[6] Due to technical difficulties implied in the functional integral approach[1] we do not touch here the question of the local-momentum fluctuation field $\{F^{(N)}(p_x)\}_{x \in \Lambda_N}$. On the other hand, the field $\tilde{F}(p_x)$, $x \in \mathbf{Z}^d$, corresponding to the Hartree–Fock approximation, which has the same global fluctuations $\tilde{F}_{\tilde{\delta}'}(p)$ as the one-component spherical model of the anharmonic crystal, can be calculated directly avoiding the functional integral approach. This calculations show that $\tilde{F}_{\tilde{\delta}}(q)$ and $\tilde{F}_{\tilde{\delta}'}(p)$ yield, for $T = 0$, $m = m_d^*$ and a properly chosen $(\tilde{\delta}, \tilde{\delta}')$, a representation of a CCR-algebra, see ref. 6. Remark that the functional integration technique could also be used in the one-component spherical model of the anharmonic crystal and raises the same technical problems at calculating the momentum fluctuations.

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