Nonuniversal critical behavior and its suppression by quantum fluctuations

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The phase transition at $T_c = 0$, caused by variation of parameters in a lattice dynamic system, is studied by means of classical and quantum-statistical mechanics. We calculate the critical exponents explicitly. They differ from those for $T_c \neq 0$. Within the frame of classical statistical mechanics they are nonuniversal, depending on a parameter. This feature is suppressed, however, by quantum fluctuations. The quantum-mechanical $T_c = 0$ critical point for a d-dimensional system corresponds to the Wilson fix point of a $(d+1)$-dimensional system.

I. INTRODUCTION

In recent years, considerable efforts have been made to investigate structural phase transitions. While in almost all cases of experimentally accessible structural phase transitions the effects of quantum mechanics do not show up in the critical behavior, there is an interesting limiting case where quantum effects play an important role, namely, at the displacive limit where the phase transition occurs at zero temperature. In the last couple of years, several papers have been concerned with the displacive limit, both theoretically[1-4] and experimentally.[5]

In this work we study the phase transition at $T_c = 0$, caused by variation of the parameters in a lattice-dynamic model for distortive phase transitions, within the framework of both classical and quantum-statistical mechanics. The $T_c = 0$ limit represents the end point of a critical line (see Fig. 1) and we shall discuss two sets of exponents describing the critical behavior as a function of temperature T and interaction strength S, respectively. In the classical treatment, we find "nonuniversal" exponents which depend on the degree of anharmonicity of the single-particle potential. This dependence disappears as soon as T_c is finite. The interesting question then arises: What happens to the zero-temperature critical exponents if the quantum-mechanical zero-point oscillations are included? The answer is the following: Quantum-mechanically, we do get "universal" exponents independent of the degree of anharmonicity. They are different, however, from the finite temperature critical exponents. We are then led to the conclusion that the universality of critical exponents is intimately connected with the presence of fluctuations either of thermal or quantum type.

Within the framework of the renormalization group, the classical displacive limit is found to correspond to a Gaussian fixed point, in contrast to the quantum case where for a d-dimensional system the displacive limit corresponds to a $(d+1)$-dimensional Wilson fixed point. In Sec. II, we will present the model Hamiltonian. Section III will be devoted to the classical treatment using the renormalization-group method adapted for the $T_c = 0$ case. In Sec. IV the quantum-mechanical displacive limit will be discussed within the framework of the $1/n$ and ϵ expansion.

II. MODEL SYSTEM AND DISPLACIVE LIMIT

In order to study the critical properties of a lattice-dynamic system, we consider the model Hamiltonian

$$\mathcal{H} = T + V_{\text{harm}} + V_{\text{anharm}} \tag{1}$$

with a kinetic energy T,

$$T = \frac{1}{2M} \sum_{l} \sum_{\alpha=1}^{n} P_{l\alpha}^2 , \tag{2}$$

and a harmonic potential energy

$$V_{\text{harm}} = \frac{A}{2} \sum_{l} \sum_{\alpha=1}^{n} X_{l\alpha}^2 - C \sum_{\langle ll' \rangle} \sum_{\alpha=1}^{n} X_{l\alpha} X_{l'\alpha} - h \sum_{l} \sum_{\alpha=1}^{n} X_{l\alpha} . \tag{3}$$

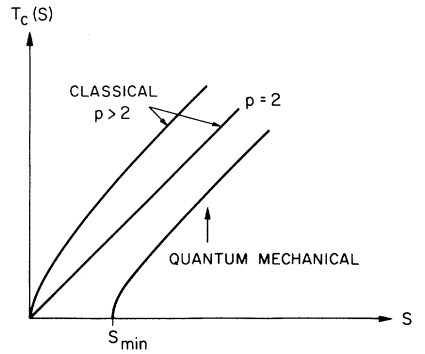

FIG. 1. Critical line of the classical and quantum-mechanical distortive model. The critical lines for $d \geq 2$ are shown for different single-particle potential parameters p.

Here, l denotes the lattice sites, $P_{l\alpha}$ and $X_{l\alpha}$ are the αth components of the n-dimensional momentum and displacement vectors. The particle mass is denoted by M. A and C are model parameters and h is a homogeneous external field. The bilinear interaction is restricted to nearest neighbors only. For the anharmonic part of the interaction we take the form

$$V_{\text{anharm}} = \frac{B_p}{2pn^{p-1}} \sum_l \left(\sum_{\alpha=1}^{n} X_{l\alpha}^2 \right)^p . \tag{4}$$

This choice differs from the usual one by the introduction of an additional parameter p which determines the form of the anharmonicity: For increasing p the potential becomes stiffer and for $p=\infty$ a rectangular shape is attained. The normalization factor is chosen such as to make the potential energy proportional to the number of components n. The Hamiltonian (1) may also be considered as a lattice model for magnetic systems where at each lattice site l there is a spin variable $\vec{X}_l$ with n components.

Recently, the phase transition at $T_c=0$, caused by variation of A and C, has been studied in the large n limit for the special case of quartic anharmonicity ($p=2$), both classically and quantum-mechanically.[1,3,4] It is the purpose of this work to extend these results to general n and to consider instead of the quartic term, anharmonicity of order $2p$ [see Eq. (4)].

In the classical treatment, the critical behavior at the displacive limit will be described by p-dependent critical exponents. This is easily seen: Using the commutation relations

$$i\hbar \dot{X}_{l\alpha} = [X_{l\alpha}, \mathcal{H}] \tag{5}$$

and

$$[X_{l\alpha}, P_{l'\alpha'}] = i\hbar \delta_{ll'} \delta_{\alpha\alpha'} , \tag{6}$$

we find from Hamiltonian (1) the equation of motion for the average values

$$-M\langle \ddot{X}_{l\alpha} \rangle = (A - 2CZ_n)\langle X_{l\alpha} \rangle + B_p \left\langle \left(\frac{1}{n} \sum_\beta X_{l\beta} \right)^{p-1} X_{l\alpha} \right\rangle - h, \tag{7}$$

where the number of nearest neighbors is denoted by Z_n. For zero external field h, it then follows that the order parameter $\langle X_{l\alpha} \rangle$ obeys the equation

$$(2CZ_n - A)\langle X_{l\alpha} \rangle = B_p \left\langle \left(\frac{1}{n} \sum_\beta X_{l\beta} \right)^{p-1} X_{l\alpha} \right\rangle . \tag{8}$$

In the large n limit this relation can be simplified considerably. First, we note that for any operator H and $G = \langle G \rangle + \delta G$ the relation

$$\langle GH \rangle = \langle G \rangle \langle H \rangle + \langle \delta G H \rangle \tag{9}$$

holds.

Defining

$$G = \frac{1}{n} \sum_\alpha X_{l\alpha}^2 , \tag{10}$$

we obtain from the Schwartz inequality

$$|\langle \delta G H \rangle|^2 \leq \langle \delta G \delta G \rangle \langle H H \rangle = O(1/n), \tag{11}$$

provided that $\langle HH \rangle$ is of order unity. This leads to

$$\langle G^{p-1} X_{l\alpha} \rangle = \langle G \rangle \langle G^{p-2} X_{l\alpha} \rangle + O(1/n^{1/2}). \tag{12}$$

So in the large n limit Eq. (8) for the order parameter becomes

$$(2CZ_n - A)\langle X_{l\alpha} \rangle = B_p \left\langle \frac{1}{n} \sum_\beta X_{l\beta}^2 \right\rangle^{p-1} \langle X_{l\alpha} \rangle , \tag{13}$$

or, equivalently,

$$\langle X_{l\alpha}^2 \rangle = [(2CZ_n - A)/B_p]^{1/(p-1)} . \tag{14}$$

Introducing the parameter

$$S = 2CZ_n - A , \tag{15}$$

this can be written as

$$\langle X_{l\alpha} \rangle^2 = (S/B_p)^{1/(p-1)} - \langle \delta X_{l\alpha}^2 \rangle . \tag{16}$$

Let us examine the $T=0$ behavior of the order parameter. Within the framework of classical statistical mechanics, there are no fluctuations at $T=0$. In this case Eq. (16) reduces to

$$\langle X_{l\alpha} \rangle_{cl} = (S/B_p)^{1/2(p-1)}; \quad T=0, \tag{17}$$

revealing the occurrence of a phase transition at $S=0$, driven by a variation of S. Clearly, the critical exponent in the S variable which will be denoted by β_S depends upon the anharmonicity parameter p. Such a phase transition also occurs in the quantum treatment, where the zero-point oscillations have to be taken into account. In fact, from Eq. (16) it follows that the order parameter will vanish at the quantum-mechanical displacive limit $S_{\min}$, defined by

$$S_{\min}/B_p = \langle \delta X_{l\alpha}^2 \rangle^{p-1} , \tag{18}$$

which does not vanish for any finite mass M and interaction strength C.

On the basis of this discussion one expects in the T-S plane, phase diagrams as sketched in Fig. 1. Provided that there is a continuous phase transition for $T=0$, the displacive limit will represent the end point of a critical line. From the previous work, where the special case of quartic anharmonicity has been treated, one expects that this end point or displacive limit represents an isolated point, with critical exponents differing from those on the critical line ($T=0$). To study these exponents and the role of the thermal and zero-point

fluctuations, we shall discuss two sets of critical exponents, describing the critical behavior as a function of temperature T for fixed S and as a function of S at fixed T, respectively. We define critical exponents along the S axis by $\chi \sim |\Delta S|^{-\gamma_S}$, $\langle X\rangle \sim |\Delta S|^{\beta_S}$, $\chi(q) \sim q^{-2+\bar{\eta}}$, $\langle X(\vec{q})X(-\vec{q})\rangle \sim q^{-2+\eta}$, and $\langle X_{1\alpha}\rangle^{\delta} \sim h$, where $\Delta_S = S - S_{\min}$. Clearly, in the classical treatment $S_{\min}$ vanishes. Along the T axis, the exponents are defined as $\chi \sim T^{-\gamma_T}$, $\chi(q) \sim q^{-2+\bar{\eta}}$, $\langle X(\vec{q})X(-\vec{q})\rangle \sim q^{-2+\eta}$, and $\langle X_{1\alpha}\rangle^{\delta} \sim h$.

III. CLASSICAL TREATMENT

In the classical case, the kinetic energy in Hamiltonian (1) can as usual be treated independently of the potential energy. Dropping the kinetic energy we may write Hamiltonian (1) in Fourier space as

$$\mathcal{H} = \sum_{\alpha} \int_0^{\Lambda} \tfrac{1}{2} M\omega^2(q) X_\alpha(q) X_\alpha(-q) d^d q + \frac{B_p}{2p n^{p-1}} \int_0^{\Lambda} d^d q \cdots \int_0^{\Lambda} d^d q\, \delta\Big(\sum_{i=1}^{2p} \vec{q}_i\Big) \sum_{\alpha_1} X_{\alpha_1}(\vec{q}_1) X_{\alpha_1}(\vec{q}_2) \cdots \sum_{\alpha_p} X_{\alpha_p}(\vec{q}_{2p-1}) \cdot X_{\alpha_p}(\vec{q}_{2p}), \tag{19}$$

where for a d-dimensional cubic system

$$M\omega_0^2(\vec{q}) = A - 4C(\cos aq_1 + \cdots + \cos aq_d). \tag{20}$$

The cutoff in the q integral is denoted by Λ, a is the lattice constant, and $q_1, \ldots, q_d$ are the components of the d-dimensional wave vector. In the low-momentum limit Eq. (20) leads to

$$M\omega_0^2(q) = -S + q^2, \tag{21}$$

where the wave numbers are measured in units of $2Ca^2$. As previously [see Eq. (15)] the parameter S is defined by

$$S = 2CZ_n - A. \tag{22}$$

In order to study the critical behavior near

$$S = 0, \quad T = 0, \tag{23}$$

we study the renormalization-group transformation

$$e^{-(\mathcal{H}/T)'} = \mathrm{Tr}' e^{-\mathcal{H}/T}. \tag{24}$$

The symbol Tr′ stands for the partial trace over the small-wavelength fluctuations of the system. The meaning of (24) for finite temperatures T is well defined and has been discussed extensively.[6-8] In order to apply the ordinary scheme of the renormalization group to the case $T_c = 0$, it is useful to introduce scaled variables $\xi_\alpha(q)$ according to

$$X_\alpha(q) = T^{1/2} \xi_\alpha(q). \tag{25}$$

In these scaled variables $\xi_\alpha(q)$ we may write

$$\frac{\mathcal{H}}{T} = \frac{1}{2} \int_0^{\Lambda} (-S + q^2) \vec{\xi}(\vec{q}) \vec{\xi}(-\vec{q}) d^d q + U_{2p} \int_0^{\Lambda} d^d q_1 \cdots \int_0^{\Lambda} d^d q_{2p}\, \delta\Big(\sum_{i=1}^{2p} \vec{q}_i\Big) \times \prod_{j=1}^{2p} [\xi(\vec{q}_{2j-1}) \cdot \vec{\xi}(q_{2j})]. \tag{26}$$

For simplicity, we have introduced a scalar product notation to indicate the summation over α. We note that in these scaled variables the anharmonicity U_{2p},

$$U_{2p} = (1/2p n^{p-1}) B_p T^{p-1}, \tag{27}$$

is temperature dependent, vanishing at $T = 0$, while the parameter of the quadratic part remains finite. We expect therefore that the displacive limit corresponds to the Gaussian fixed point. In order to calculate the renormalization transformation (24) we separate the Hamiltonian (26) into an effective quadratic part

$$\frac{\mathcal{H}_0}{T} = \frac{1}{2} \int_0^{\Lambda} (r + q^2) \vec{\xi}(\vec{q}) \vec{\xi}(-\vec{q}) d^d q, \tag{28}$$

and an interaction term

$$\frac{\mathcal{H}_{\mathrm{int}}}{T} = \frac{1}{2} \int_0^{\Lambda} (-S - r) \vec{\xi}(\vec{q}) \vec{\xi}(-\vec{q}) d^d q + U_{2p} \int_0^{\Lambda} d^d q_1 \cdots \int_0^{\Lambda} d^d q_{2p} \delta\Big(\sum_{i=1}^{2p} \vec{q}_i\Big) \times \prod_{i=1}^{p} [\vec{\xi}(q_{2i-1}) \vec{\xi}(\vec{q}_{2i})], \tag{29}$$

and use the usual power-series expansion in $\mathcal{H}_{\mathrm{int}}$,[6]

$$e^{-(\mathcal{H}/T)'} = \mathop{\mathrm{Tr}}_{\Lambda/b < q < \Lambda} e^{-\mathcal{H}_0/T} e^{-\mathcal{H}_{\mathrm{int}}/T} = \mathop{\mathrm{Tr}}_{\Lambda/b < q < \Lambda} e^{-\mathcal{H}_0/T} (1 - \mathcal{H}_{\mathrm{int}}/T + \tfrac{1}{2}\mathcal{H}_{\mathrm{int}}^2/T^2 - + \cdots). \tag{30}$$

Here, $\mathcal{H}_0$ is chosen such that the linear term in $\mathcal{H}_{\mathrm{int}}$ does not give rise to a renormalization of r. This leads to

$$r = \mathrm{const}\, U_{2p} + O(U_{2p}^2). \tag{31}$$

Evaluating the partial trace in (30) leads then to the recursion relations[6]

$$r' = b^2[r + O(U_{2p}^2)], \tag{32}$$

$$U_{2p}' = b^{p(2-d)+d}[U_{2p} + O(U_{2p}^2)]. \tag{33}$$

In contrast to the usual case for finite T, our U_{2p}

is explicitly temperature dependent, vanishing at the displacive limit. Thus, the displacive limit is represented by the Gaussian fixed point of Eqs. (32) and (33) and r and U_{2p} may be considered as the perturbations around this fixed point. We have to distinguish the cases $d>2$ and $d<2$. For dimensionalities $d>2$, r will always be the more relevant perturbation. Owing to (31) together with (27) we have

$$r \propto T^{p-1}. \tag{34}$$

Thus, for $S=0$ and B_p fixed, we obtain a recursion for the temperature

$$T' = b^{2/(p-1)}T + O(T^{p-1}); \quad d>2, \tag{35}$$

which according to[6]

$$\nu = \ln b/\ln b^s = 1/s, \tag{36}$$

leads to

$$\nu_T = \tfrac{1}{2}(p-1); \quad d>2, \tag{37}$$

and as for a Gaussian fixed point $\eta=0$,

$$\gamma_T = 2\nu_T = p-1; \quad d>2. \tag{38}$$

On the other hand, for dimensionalities $d<2$, U_{2p} is the more relevant perturbation. Owing to (27), for fixed B_p, this leads to a recursion for the temperature T

$$T' = b^{(p(2-d)+d)/(p-1)}[T + O(T^{p-1})]; \quad d<2. \tag{39}$$

Thus, for $d<2$, we obtain

$$\nu_T = (p-1)/[p(2-d)+d]; \quad d<2, \tag{40}$$

and

$$\gamma_T = 2\nu_T = 2(p-1)/[p(2-d)+d]; \quad d<2. \tag{41}$$

For the sake of completeness, we also list the $T=0$ critical exponents, which are of course mean-field-like. They are

$$\nu_s = \tfrac{1}{2}, \quad \eta = 0, \quad \beta_s = 1/2(p-1); \quad \delta = 2p-1, \quad \gamma_s = 1. \tag{42}$$

All these exponents are clearly independent of the number of components n of the order parameter and for the special case of a quartic potential they adopt the values that have been previously obtained.[1-4]

IV. QUANTUM-MECHANICAL TREATMENT

In order to study the modifications of the critical behavior of our lattice-dynamic model due to quantum effects we have to evaluate the quantum mechanical partition function. For this purpose we make use of Feynman's path integral technique.[9] Let us briefly review the essential features of this method on the basis of the Hamiltonian

$$\mathcal{H} = \tfrac{1}{2}m\dot{X}^2 + V(X). \tag{43}$$

The density matrix $\rho(X,X';\beta)$ at an inverse temperature $\beta = 1/kT$ is then written as an integral over all paths connecting the points X and X' as

$$\rho(X,X';\beta) = \int \exp\left(-\frac{1}{\hbar}\int_0^{\beta\hbar}\{\tfrac{1}{2}m\dot{X}^2(\tau) + V[X(\tau)]\}d\tau\right)\mathfrak{D}X(\tau), \tag{44}$$

$$X(0) = X,$$

$$X(\beta\hbar) = X',$$

and the partition function Z is given by

$$Z(\beta) = \int \rho(X,X';\beta)dX. \tag{45}$$

Using the Fourier representation (19) we can write Hamiltonian (1), which now includes the kinetic energy, as

$$\mathcal{H} = \sum_\alpha \int_0^\Lambda d^d q\, \tfrac{1}{2}M[\dot{X}_\alpha(q,t)\dot{X}_\alpha(-q,t) + \omega_0^2(q)X_\alpha(q,t)X_\alpha(-q,t)]$$
$$+ \frac{B_p}{2pn^{p-1}}\int_0^\Lambda d^d q_1 \cdots \int_0^\Lambda d^d q_{2p}\,\delta\left(\sum_{i=1}^{2p}\vec{q}_i\right)\prod_{j=1}^{p}\left(\sum_\alpha X_\alpha(\vec{q}_{2j-1},t)X_\alpha(\vec{q}_{2j},t)\right). \tag{46}$$

Here, we have used the definition (20) for $\omega_0^2(q)$ and $\dot{X}$ is the velocity operator.

In order to carry out the τ integral in (44) it is useful to introduce a discrete Fourier representation of $X_\alpha(\vec{q},t)$ defined for $0<\tau<\beta\hbar$,

$$X_\alpha(\vec{q},\tau) = \sum_{\nu=-\infty}^{\infty} X_\alpha(\vec{q},\omega_\nu)e^{i\omega_\nu\tau}. \tag{47}$$

The Matsubara frequency ω_ν is given by

$$\omega_\nu = 2\pi\nu/\beta\hbar. \tag{48}$$

Carrying out the τ integration [see Eq. (44)] we obtain

$$\Phi(\beta)=\frac{1}{\hbar}\int_0^{\beta\hbar}\mathcal{H}d\tau=\beta\left[\frac{M}{2}\sum_{q,\nu,\alpha}\{[\omega_\nu^2+\omega_0^2(q)]X_\alpha(q,\omega_\nu)X_\alpha(-q,-\omega_\nu)\}+\frac{B_p}{2pn^{p-1}}\right.$$
$$\left.\times\sum_{\substack{q_1\cdots q_{2p}\\ \omega_1\cdots\omega_{2p}}}\delta\Big(\sum\vec{q}_i\Big)\,\delta\Big(\sum\omega_i\Big)\prod_{j=1}^{p}\Big(\sum_\alpha X_\alpha(q_{2j-1},\omega_{2j-1})X_\alpha(q_{2j},\omega_{2j})\Big)\right]. \tag{49}$$

For the sake of simplicity the q integrals are written as sums. The partition function is now obtained by integrating over all Fourier components[9] $X_\alpha(q,\omega_\nu)$:

$$Z=\int J\prod_{q,\nu,\alpha}dX_\alpha(q,\omega_\nu)e^{-\Phi(\beta)}. \tag{50}$$

The symbol J denotes the Jacobian which comes from the change of variables $\mathfrak{D}X(\tau)$ to $\prod_\nu dX(\omega_\nu)$, it does not depend upon the dynamics of the system.[10]

For the following, it is useful to separate $\Phi(\beta)$ into a harmonic part $\Phi_0(\beta)$,

$$\Phi_0(\beta)=\tfrac{1}{2}M\beta\sum_{q,\nu,\alpha}[\omega_\nu^2+\omega_0^2(q)]X_\alpha(q,\omega_\nu)X_\alpha(-q,-\omega_\nu), \tag{51}$$

and an anharmonic part, which for the quartic case looks like

$$\Phi_I(\beta)=\beta\frac{u_4}{4n}\sum_{\substack{q_1q_2q_3\\ \omega_1\omega_2\omega_3}}\sum_{\alpha\beta}X_\alpha(q_1,\omega_1)X_\alpha(q_2,\omega_2)$$
$$\times X_\beta(q_3,\omega_3)X_\beta\Big(-\sum q_i,-\sum\omega_i\Big). \tag{52}$$

The partition function can then be represented as

$$Z=Z_0\langle e^{-\Phi_I(\beta)}\rangle, \tag{53}$$

where the average $\langle A\rangle_0$ is defined by

$$\langle A\rangle_0=\int e^{-\Phi_0(\beta)}A\Big/\int e^{-\Phi_0(\beta)}. \tag{54}$$

We will now use this expression to calculate the critical behavior of this system in both ϵ and $1/n$ expansion.

A. Zero-temperature critical behavior

We note that for $T\to 0$ the Matsubara frequencies (48) form a continuum and therefore play the role of an additional wave vector q_{d+1},

$$q_{d+1}=\omega_\nu. \tag{55}$$

As a consequence, the zero-temperature critical behavior of this d-dimensional system is thus equivalent to a $(d+1)$-dimensional Ginzburg-Landau-Wilson system[6] for which the critical behavior is known to be described by

$$\nu_S=\tfrac{1}{2}+[(n+2)/4(n+8)]\epsilon;\quad d<3$$
$$\nu_S=\tfrac{1}{2};\quad d>3 \tag{56}$$

and

$$\gamma_S=1+[n+2/2(n+8)]\epsilon;\quad d<3$$
$$\gamma_S=1;\quad d>3. \tag{57}$$

In our case ϵ is given by

$$\epsilon=3-d. \tag{58}$$

Moreover, $d=3$ represents the borderline between mean-field and nonclassical behavior. The subscript S in (56) and (57) refers to the fact that at zero temperature the phase transition is driven by variation of S. We note that while the classical displacive limit corresponds to the Gaussian fixed point for all spatial dimensionalities, the quantum-mechanical zero-temperature fixed point is Gaussian only above three dimensions. Furthermore, the reason for anharmonicity-dependent exponents in the classical case stems from the fact that in the recursion high-order anharmonicity does not produce lower-order terms. This is in contrast to the Wilson case at finite temperature and to the quantum-mechanical zero-temperature situation. In the latter case the zero-point fluctuations destroy the anharmonicity effects on the critical exponents.

Approaching the $T=0$ fixed point from finite temperatures the situation is changed considerably: For finite temperature the Matsubara frequencies have a finite spacing and the d-dimensional quantum system resembles a $(d+1)$-dimensional classical system which is finite in one dimension. Within the framework of the renormalization-group recursion relations this gives rise to a dimensional crossover problem. We refer the reader to the paper by Hertz,[11] who discusses recursion relations where the expansion parameter ϵ depends on the recursion step.

B. Large-n limit and $1/n$ corrections

As mentioned above, the approach of the zero-temperature critical point from finite temperatures is associated with a dimensional crossover. Finite-size scaling theory[12] might be applied to this problem.

We first review briefly the $n=\infty$ limit.[3,7,12] The large n-limit results are obtained by decomposing $\Phi(\beta)$ from Eq. (49) into an effective harmonic part (Hartree part) $\Phi_{SC}(\beta)$,

$$\Phi_{SC}(\beta)=\beta\left[\frac{1}{2}\sum_{\alpha q\nu}\left(-S+q^2+M\omega_\nu^2+\frac{n+2}{n}u_4\langle X^2\rangle_{SC}\right)|X_\alpha(q,\omega_\nu)|^2\right] \tag{59}$$

and an anharmonic part

$$\Phi_I(\beta)=\frac{\beta U_4}{4n}\left[\sum_{\substack{q_1q_2q_3\\ \omega_1\omega_2\omega_3\\ \alpha,\beta}} X_\alpha(q_1\omega_1)X_\alpha(q_2\omega_2)X_\beta(q_3\omega_3)X_\beta\left(-\sum q_i,-\sum\omega_i\right)-2(n+2)\langle X^2\rangle_{SC}\sum_{q\omega_\nu\alpha}X_\alpha(q,\omega_\nu)X_\alpha(-q,-\omega_\nu)\right], \tag{60}$$

such that $\Phi_I(\beta)$ gives no contribution in the limit $n\to\infty$. The harmonic part is, as usual, determined by a self-consistency equation. Denoting averages with respect to $\Phi_{SC}(\beta)$ by $\langle\ \rangle_{SC}$ one obtains

$$\langle|X_\alpha(q,\omega_\nu)|^2\rangle_{SC}=\frac{kT}{-S+q^2+M\omega_\nu^2+[(n+2)/n]u_4\langle X^2\rangle_{SC}} \tag{61}$$

and summing over the Matsubara frequency, we obtain a self-consistency equation for $\langle X^2\rangle_{SC}$,

$$\langle X^2\rangle_{SC}=kT\sum_{\nu,q}\frac{1}{-S+q^2+M\omega_\nu^2+[(n+2)/n]u_4\langle X^2\rangle_{SC}}. \tag{62}$$

Introducing a renormalized coupling strength

$$r=-S+[(n+2/n]u_4\langle X^2\rangle_{SC}, \tag{63}$$

the condition of self-consistency becomes

$$r+S=\frac{n}{n+2}u_4kT\sum_q\sum_{\nu=\infty}^{+\infty}\frac{1}{r+q^2+M\omega_\nu^2}, \tag{64}$$

where the renormalized propagator

$$G(q,\omega_\nu)=1/(r+q^2+M\omega_\nu^2), \tag{65}$$

differs from the classical one by the appearance of an additional "wave vector" ω_ν which for $T\to0$ leads to the dimensional crossover discussed previously. All the well-known techniques for calculating the $1/n$ expansion can now be applied with the only difference that for finite T one of the wave vectors is a discrete variable. Furthermore we note that the retarded response function $\chi(q,\omega)$ is obtained from $G(q,\omega_\nu)$ by analytic continuation from the imaginary frequency axis to the real one. For the static susceptibility this leads to

$$\chi(q,\omega=0)=1/(r+q^2). \tag{66}$$

Let us first examine the critical line $T_c(S)$ which is defined by the condition $r=0$. Summing over the Matsubara frequencies and integrating over the wave vectors in Eq. (64) leads to

$$r+S=\tfrac{1}{2}u_4\int_0^\Lambda q^{d-1}\frac{\hbar}{[(r+q^2)M]^{1/2}}\times\coth\frac{\hbar[(r+q^2)/M]^{1/2}}{2kT}\,dq. \tag{67}$$

For convenience we set $\hbar=M=1$. The q integral can be separated into a zero-temperature part

$$K_0(r)=\frac{1}{2}\int_0^\Lambda q^{d-1}\frac{1}{(r+q^2)^{1/2}}\,dq \tag{68}$$

and a finite temperature contribution

$$K_1(r,T)=\int_0^\Lambda q^{d-1}\frac{1}{(r+q^2)^{1/2}}\frac{1}{\exp[(r+q^2)^{1/2}/kT]-1}\,dq \tag{69}$$

whose leading low-T behavior is given by[3]

$$K_1(r,T)\sim T^{d-1}\Phi(r/T^2), \tag{70}$$

with

$$\Phi(X)=\int_0^\infty dt\,\frac{t^{d-1}}{(X+t^2)^{1/2}[\exp(X+t^2)^{1/2}-1]} \tag{71}$$

and $\Phi(0)$ is a finite constant. The self-consistency Eq. (66) can now be cast into the form

$$r+S=\tfrac{1}{2}u_4[K_0(r)+T^{d-1}\Phi(r/T^2)]. \tag{72}$$

The critical line $T_c(S)$ has thus the asymptotic form

$$T_c(S)\sim(S-S_{\min})^{1/(d-1)}, \tag{73}$$

where $S_{\min}$ is connected with $K_0(r=0)$ by

$$S_{\min}=\tfrac{1}{4}u_4K_0(0) \tag{74}$$

which for dimensions $d>1$ has a finite-positive value. For $d=1$, however, it goes to infinity,[4] showing that in the large-n limit a one-dimensional system does not undergo a phase transition even at zero temperature. For dimensions $d>2$ the critical line has an infinite slope. Thus, the critical behavior along the line $S=S_{\min}$ described by exponents γ_T, ν_T, etc., will differ from the one along the line $T=0$, which is driven by variation of S.

To study this further, let us investigate the property of $G(q,\omega_\nu)$ along the line $S=S_{\min}$ and calculate the self-energy r as a function of temperature. For this purpose we calculate the small-r behavior of $K_0(r)$,[3]

$$K_0(r)\sim K_0(0)-\begin{cases}dr+br^{(d-1)/2}; & 1<d<3\\ dr+br\ln r; & d=3\\ dr+\cdots; & d>3.\end{cases} \tag{75}$$

The self-consistency equation (72) thus shows that

along the line $S=S_{\min}$ r varies as

$$r\sim T^2;\quad 1<d<3 \tag{76}$$

and

$$r\sim T^{d-1};\quad d>3, \tag{77}$$

while at $T=0$, r behaves as

$$r\sim (S-S_{\min})^{2/(d-1)};\quad 1<d<3 \tag{78}$$

and

$$r\sim S-S_{\min};\quad d>3\,. \tag{79}$$

From Eq. (66) for the static susceptibility we thus obtain in the large-n limit

$$\gamma_T=2,\quad \gamma_S=2/(d-1);\quad 1<d\leq 3 \tag{80}$$

and

$$\gamma_T=d-1,\quad \gamma_S=1;\quad d>3, \tag{81}$$

with logarithmic corrections for $d=3$. Similarly, defining the correction length by

$$\xi^2=-\left(\frac{1}{\chi(q,0)}\,\frac{d^2\chi(q,0)}{dq^2}\right)_{q=0}, \tag{82}$$

we obtain

$$\nu_T=\tfrac{1}{2}\gamma_T \quad\text{and}\quad \nu_S=\tfrac{1}{2}\gamma_S\,. \tag{83}$$

From Eqs. (80) and (81) the shift exponent ψ is found to be

$$\psi=\gamma_T/\gamma_S=d-1 \tag{84}$$

in agreement with the expression (73) for the critical line.

Let us now determine the $1/n$ corrections to the critical exponents at zero temperature. Clearly, the results obtained for classical systems can be applied to our case and again the appearance of the Matsubara frequencies in the propagator lead to an effective rise of the dimensionality by one unit. To order $1/n$ the propagator $G^{(1)}(q,\omega_\nu)$ is given by[13-15]

$$G^{(1)}(q,\omega_\nu)=G(q,\omega_\nu)-2G^2(q,\omega_\nu)u_4\beta/n \times\sum_{q'\omega_\nu'}\frac{G(q'-q,\omega_\nu')}{1+\beta u_4\Pi_0(q',\omega_\nu')}\,, \tag{85}$$

where

$$\Pi_0(q,\omega_\nu)=\sum_{q'\omega_\nu'}G(q',\omega_\nu')G(q-q',\omega_\nu-\omega_\nu')\,. \tag{86}$$

This leads to zero-temperature critical exponents

$$\gamma_S=\frac{2}{d-1}-\frac{6}{n}\,\frac{\sin[(d+1)\frac{1}{2}\pi]\Gamma(d)}{(1-d)\pi[\Gamma(\frac{1}{2}(d+1))]^2}+O\left(\frac{1}{n^2}\right) \tag{87}$$

or introducing $d=3-\epsilon$

$$\gamma_S=1+\tfrac{1}{2}\epsilon-3\epsilon/n\,, \tag{88}$$

which to order $1/n$ agrees with the ϵ-expansion result (57). Similarly defining the critical exponent η by

$$G^{(1)}(q,0)\sim 1/q^{2-\eta}, \tag{89}$$

we obtain to order $1/n$

$$\eta=\frac{1}{n}\left(\frac{8}{(d+1)}-2\right)\frac{1}{\pi}\,\sin[\pi\tfrac{1}{2}(d-1)]\Gamma(d)/\Gamma^2(\tfrac{1}{2}(d+1))\,. \tag{90}$$

These results, valid on the S axis at $T=0$, are easily generalized to the line $S=S_{\min}$ where the critical point is approached from finite temperature. From Eqs. (76)–(79) we see that for all dimensions $d>1$ in the propagator (65) there is an exact correspondence between the variable $\Delta S=S-S_{\min}$ at zero temperature and the variable T^{d-1} for $S=S_{\min}$. So we conclude that for all orders in $1/n$ we have the relation

$$\gamma_T=(d-1)\gamma_S \tag{91}$$

and

$$\nu_T=(d-1)\nu_S\,. \tag{92}$$

This same argument is also valid for the diagrammatic ϵ expansion.[6,15] Thus, from (56) and (57) we obtain to order ϵ

$$\nu_T=1-[3/(n+8)]\epsilon \tag{93}$$

and

$$\gamma_T=2-[6/(n+8)]\epsilon\,. \tag{94}$$

So far, we have restricted the discussion of the quantum-mechanical displacive limit to quartic anharmonicity only. The case of higher-order anharmonicity can be handled in the same way. Like for classical $(d+1)$-dimensional systems, this will give rise to tricritical phenomena but no anharmonicity-dependent critical exponents.

V. CONCLUSIONS

We have studied the critical behavior of lattice-dynamical systems at $T_c=0$, caused by variation of parameters. In the classical case, "nonuniversal" exponents which depend on the degree of anharmonicity of the single-particle potential are found. They do not depend on the number of components n. If quantum fluctuations are taken into account, however, the critical exponents for a d-dimensional system correspond to the Wilson exponents of a $(d+1)$-dimensional classical system.

For finite temperatures the system becomes finite in this extra dimension and the resulting finite-size effect gives rise to dimensional crossover phenomena. While in the large-n limit for one-dimensional systems the phase transition at

zero temperature is suppressed by quantum fluctuations, one may still expect critical behavior for the quantum cases $n=1$, $d=1$ and $n=2$, $d=1$, which, according to our formulation, correspond to a two-dimensional classical Ising model and XY model, respectively. The divergence of $S_{\min}$ for $n=\infty$ and $d=1$ is a consequence of $\eta=0$. As for the two-dimensional Ising model η is larger than zero the value of $S_{\min}$ may remain finite for the one-dimensional one-component system.

From our formulation it also follows that the $T=0$ phase transition of any lattice dynamical systems will be described by the appropriate $(d+1)$-dimensional Wilson fixed point, provided that the inverse of the propagator is quadratic or bilinear in the wave-vector components. Clearly, this also includes dipolar interactions which are relevant for ferroelectric systems.

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