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Quantum effects in an n-component vector model for structural phase transitions

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The influence of quantum effects on the critical properties of an n-component vector model for structural phase transitions is explored. It is shown for $n = 1$, 2, and ∞ that these effects can suppress the occurrence of a phase transition for all dimensions d. This turns out to be of particular relevance for systems where the classical transition temperature almost vanishes ($T_c = 0$ represents the displacive limit). We also discuss the critical properties at this limit for $n = \infty$ and show that the critical exponents change discontinously.

I. INTRODUCTION

The static and dynamic properties of model systems undergoing a structural phase transition have been studied recently by a number of authors, with emphasis on the critical behavior.[1–12] One of the reasons for this interest is that many real systems undergo a structural phase transition which takes the system from a high-temperature displacement pattern to a different low-temperature displacement configuration. To imitate such systems one may adopt the Hamiltonian

$$\mathcal{H} = \sum_{L,\alpha} \frac{P_{L\alpha}^2}{2M} + \frac{A}{2} \sum_{L,\alpha} X_{L\alpha}^2 + \frac{B}{4n} \sum_L \Big(\sum_\alpha X_{L\alpha}^2 \Big)^2 - C \sum_{L,L',\alpha} X_{L\alpha} X_{L'\alpha} - h \sum_{L,\alpha} X_{L\alpha} \quad . \qquad (1)$$

L denotes the lattice sites and $P_{L\alpha}$ and $X_{L\alpha}$ are the αth components ($\alpha = 1, \cdots, n$) of momentum and displacement, respectively, of particles with mass M. A, B, and C are model parameters and h is an external field. Higher-order terms $\sum_L (\sum_\alpha X_{L\alpha'}^2)^3$, etc. may give rise to tricritical points.[13–15] Neglecting the kinetic energy, Hamiltonian (1) may also be considered as a lattice model for magnetic systems, where at each site L, there is a spin variable $\vec{X}_L$ with n components.[16,17]

In recent years, the static and dynamic properties of these systems have been studied by means of different techniques. They include the renormalization-group approach,[2,6,16] the Monte Carlo,[18] and the molecular-dynamics technique.[3–5,11] Even exact results have been established for quartic long-range interactions[10,14] and in the limit $n \to \infty$,[9,15,17] as well as for the existence of a phase transition.[19]

A common feature of these studies is the use of classical mechanics. Quantum effects can no longer be neglected, however, if the model parameters are such that the classical zero-temperature value of the order parameter becomes very small or even vanishes. Indeed one expects that the occurrence of a phase transition will be suppressed, if the local mean-square displacement fluctuation $\langle \delta X_{L\alpha}\, \delta X_{L\alpha} \rangle$ becomes equal or larger than the classical value of the zero-temperature order parameter squared.

It is the purpose of this work to investigate the influence of quantum effects on the occurrence of a phase transition and on the critical properties.

In Sec. II, we derive an exact inequality, demonstrating that zero-point oscillations can suppress the occurrence of a phase transition. This effect is shown to be particularly relevant for systems having model parameters close to the classical displacive limit, which represents an isolated point with different critical exponents.[20–22] In fact, we establish for $n = 1$, 2, and ∞ and all dimensionalities d that zero-point fluctuations will suppress a phase transition at this limit. Moreover, we find a quantum-mechanical displacive limit, i.e., a particular choice of the model parameters for which T_c vanishes.

The limit $n = \infty$ is treated in Sec. III, where we investigate the critical properties, including those at the quantum-mechnical displacive limit. We find, at least for $n = \infty$, that this limit also represents an isolated point, where the critical exponents change discontinuously. For $T_c \neq 0$ the exponents are equal to those of the spherical model, where $\gamma = 2/(d-2)$ and $\delta = (d+2)/(d-2)$ for dimensionality $2 < d \leq 4$. For $d \leq 2$, there is no phase transition. At the quantum-mechnical displacive limit, where $T_c = 0$, we find $\delta = (d+3)/(d-1)$ for $1 < d < 3$, $\delta = 3$ for $d \geq 3$, as well as $\gamma = 2$ for $1 < d \leq 3$, and $\gamma = d - 1$ for $d > 3$. These differences reveal that the quantum-mechanical displacive limit also represents an isolated point giving rise to crossover phenomena. It also follows that the mean-field domain for δ ranges down to $d = 3$ at the quantum-mechanical displacive limit, in contrast to the usual case of $d = 4$.

In Sec. IV, the main results are summarized and implications to real systems are discussed.

II. DEFINITIONS AND DERIVATION OF AN INEQUALITY

In this section, we derive relations between the local mean-square displacement and the model parameters. On this basis, we establish the suppression of a phase transition due to zero-point oscillations.

To simplify the derivation, we adopt the Hamiltonian (1) describing ferrodistortive structural phase transitions. The rigid reference lattice is assumed to be cubic, with $2d$ nearest neighbors. Only nearest-neighbor interactions are taken into account. Using the relations

$$i\hbar \dot{X}_{L\alpha} = [X_{L\alpha}, \mathcal{H}] \quad , \tag{2}$$

$$[X_{L\alpha}, P_{L'\alpha'}] = \delta_{LL'}\delta_{\alpha\alpha'} i\hbar \quad , \tag{3}$$

we find

$$-\langle \dot{P}_{L\alpha}\rangle = -m\langle \ddot{X}_{L\alpha}\rangle = (A-4dC)\langle X_{L\alpha}\rangle + B\left\langle \frac{1}{n}\sum_{\beta=1}^{n} X_{L\beta}^2 X_{L\alpha}\right\rangle - h = 0 . \tag{4}$$

For zero external field, it then follows that

$$\frac{4dC-A}{B}\langle X_{L\alpha}\rangle = \left\langle \frac{1}{n}\left(\sum_{\beta=1}^{n} X_{L\beta}^2\right) X_{L\alpha}\right\rangle \quad . \tag{5}$$

Within the framework of classical mechanics, there are no fluctuations at zero temperature. In this case, relation (5) reduces to

$$\frac{4dC-A}{B} = \langle X_{L\alpha}\rangle^2_{\mathrm{cl}, T=0} \quad , \tag{6}$$

and determines the zero-temperature values of the order parameter. There are two important limits[5]: (i) the displacive limit where

$$4dC - A = 0 \quad \text{(displacive limit)} \ , \tag{7}$$

so that the classically determined order parameter vanishes even at $T=0$. (ii) The Ising limit, where

$$A=-\infty, \quad B=+\infty, \quad A/B=-1 \quad \text{(Ising limit)}. \tag{8}$$

Here $\langle X_{L\alpha}\rangle^2 = 1$. Consequently, we may distinguish two regimes.[5] The choice,

$$A<0, \quad B>0, \quad C>0 \quad , \tag{9}$$

leads to transitions of the order-disorder type and

$$A>0, \quad B>0, \quad C>0, \text{ and } 4dC-A>0 \tag{10}$$

to displacive transitions. For further details on this nomenclature and its relevance to characterize real systems, we refer to Ref. 5.

The model parameter dependence of the classical zero-temperature value of the order parameter has two important consequences: (a) The classically calculated spontaneous order parameter vanishes at the displacive limit for all temperatures. (b) The classical displacive limit represents, in the space of the model parameters, an isolated point in the sense that the critical exponents change discontinuously.[20–22]

The vanishing classical transition temperature implies, however, that physical reality may be different in any lattice-dynamical system, due to the existence of zero-point oscillations. To establish this conjecture, we note that the inequality,

$$\left\langle \frac{1}{n}\left(\sum_{\beta=1}^{n} X_{L\beta}^2\right) X_{L\alpha}\right\rangle \ge \left\langle \frac{1}{n}\sum_{\beta=1}^{n} X_{L\beta}^2\right\rangle \langle X_{L\alpha}\rangle \ , \tag{11}$$

holds for $n=1, 2$, and in the limit $n=\infty$ as an equality. This relation is an extension of a Griffiths-Kelly-Sherman inequality[23–25] to quantum-mechanical and lattice-dynamical systems. The derivation of this inequality will be given in Appendix A.

From Eq. (5) and inequality (11) it then follows

$$\left[\frac{4dC-A}{B} - \frac{1}{n}\sum_{\beta=1}^{n}\langle \delta X_{L\beta}^2\rangle\right]\langle X_{L\alpha}\rangle \ge \langle X_{L\alpha}\rangle^3 \ . \tag{12}$$

Consequently, a nonvanishing positive order parameter requires that

$$\frac{4dC-A}{B} > \frac{1}{n}\sum_{\beta=1}^{n}\langle \delta X_{L\beta}^2\rangle \ . \tag{13}$$

Due to zero-point oscillations, the local mean-square displacement fluctuations $\langle \delta X_{L\alpha}^2\rangle$ do not vanish at $T=0$ for any finite mass M of the particles. It then follows that an ordered state ($\langle X_{L\alpha}\rangle \neq 0$) is suppressed if at $T=0$,

$$\frac{4dC-A}{B} \le \frac{1}{n}\sum_{\beta=1}^{n}\langle \delta X_{L\beta}^2\rangle \ . \tag{14}$$

Consequently for any physically meaningful mass M, there exists a quantity $S_{\min}$ defined by

$$\frac{S_{\min}}{B} = \frac{1}{n}\left\langle \sum_{\beta=1}^{n} \delta X_{L\beta}^2\right\rangle \ , \tag{15}$$

so that for model parameters satisfying

$$4dC - A = S_{\min} \quad , \tag{16}$$

the quantum-mechanical displacive limit is reached, where, according to inequality (12), $\langle X_{L\alpha}\rangle = 0$ even at $T=0$.

From the results presented in this section, the following conclusions may be drawn. Zero-point fluctuations may suppress the occurrence of an ordered state. This result is particularly relevant for systems having model parameters close to the classical displacive limit ($4dC-A \lesssim 0$). In fact here, zero-point oscillations can suppress the phase transition.

According to the range of validity of inequality (11), these results are rigourous for all values of the dimensionality d for $n=1, 2$ and $n=\infty$.

Unfortunately, the proof of inequality (11) has not yet been extended to systems with $2<n<\infty$. On this basis it is impossible, however, to study the critical properties at the quantum-mechanical displacive limit, in order to find a possible discontinuous change of the critical exponents and associated crossover phenomena.

To explore these questions, we study in the next section the limit $n\to\infty$ which can be treated exactly.

III. LARGE-n LIMIT

It is quite straightforward to study the static properties of model Hamiltonian (2) in the limit $n\to\infty$. First, we note that Eq. (5) reduces to

$$\frac{4dC-A}{B}\langle X_{L\alpha}\rangle=\frac{1}{n}\sum_{\beta=1}^{n}\langle X_{L\beta}^2\rangle\langle X_{L\alpha}\rangle , \tag{17}$$

because

$$\left\langle\frac{1}{n}\sum_{\beta=1}^{n}X_{L\beta}^2X_{L\alpha}\right\rangle=\langle GX_{L\alpha}\rangle=\langle G\rangle\langle X_{L\alpha}\rangle+\langle\delta G\delta X_{L\alpha}\rangle , \tag{18}$$

and

$$\langle\delta G\delta X_{L\alpha}\rangle^2\leq\langle\delta G\delta G\rangle\langle\delta X_{L\alpha}\delta X_{L\alpha}\rangle, \tag{19}$$

where

$$\langle\delta G\delta G\rangle=O(1/n) . \tag{20}$$

Rewriting Eq. (17) in the form

$$\left(\frac{4dC-A}{B}-\frac{1}{n}\sum_{\beta=1}^{n}\langle\delta X_{L\beta}^2\rangle\right)\langle X_{L\alpha}\rangle=\langle X_{L\alpha}\rangle^3 , \tag{21}$$

it is seen that inequality (13) holds in the limit $n=\infty$ as an equality. It again leads to condition (15) for the suppression of an ordered phase and to relation (16) defining the quantum-mechanical displacive limit, where the order parameter vanishes.

To study the critical properties of the $n=\infty$ model at this limit, we start from the equation of motion,

$$\begin{aligned}-M\langle\ddot{X}_{L\alpha}(t)X_{L'\alpha}(0)\rangle&=A\langle X_{L\alpha}(t)X_{L'\alpha}(0)\rangle\\&+\frac{B}{n}\left\langle\sum_{\beta=1}^{n}X_{L\beta}^2(t)X_{L\alpha}(t)X_{L'\alpha}(0)\right\rangle\\&-2C\sum_{L''}\langle X_{L''\alpha}(t)X_{L'\alpha}(0)\rangle .\end{aligned} \tag{22}$$

In the limit $n\to\infty$, the second term on the right-hand side simplifies according to Eqs. (18)–(20) to

$$\begin{aligned}&\frac{B}{n}\left\langle\sum_{\beta=1}^{n}X_{L\beta}^2(t)X_{L\alpha}(t)X_{L'\alpha}(0)\right\rangle\\&=\frac{B}{n}\sum_{\beta=1}^{n}\langle X_{L\beta}^2\rangle\langle X_{L\alpha}(t)X_{L'\alpha}(0)\rangle .\end{aligned} \tag{23}$$

Thus the spectral function

$$\Phi_{\alpha\alpha}(\vec{q},t)=\langle[X_\alpha(-\vec{q},0), X_\alpha(\vec{q},t)]\rangle , \tag{24}$$

with

$$X_\alpha(\vec{q},t)=\frac{1}{\sqrt{N}}\sum_L\delta X_{L\alpha}(t)e^{i\vec{q}\cdot\vec{R}_L} \tag{25}$$

has harmonic time dependence

$$-\ddot{\Phi}_{\alpha\alpha}(\vec{q},t)=\omega^2(\vec{q})\Phi_{\alpha\alpha}(\vec{q},t) , \tag{26}$$

with frequency

$$M\omega^2(\vec{q})=A-4CF(\vec{q})+\frac{B}{n}\sum_\beta\langle X_{L\beta}^2\rangle , \tag{27}$$

where for $d=3$

$$F(\vec{q})=\cos q_ya+\cos q_ya+\cos q_za . \tag{28}$$

Thus for $n=\infty$, the dynamics is described by temperature-dependent undamped modes so that the self-consistent phonon approximation becomes exact.

Next, the wave-vector-dependent dynamic susceptibility,

$$\chi_{\alpha\alpha}(\vec{q},\omega)=i\lim_{\epsilon\to0^+}\int_0^\infty dt\,e^{i(\omega+i\epsilon)t}\,\Phi_{\alpha\alpha}(\vec{q},t) \tag{29}$$

is calculated to be

$$\chi_{\alpha\alpha}(\vec{q},\omega)=-\frac{1}{M}\frac{1}{(\omega+i\epsilon)^2-\omega^2(\vec{q})} . \tag{30}$$

At $T=T_c$, the zero-frequency susceptibility diverges, so that according to Eqs. (27) and (30)

$$\begin{aligned}&\chi_{\alpha\alpha}^{-1}(\vec{0},0)=M\omega^2(\vec{0})\\&=A-4dC+\frac{B}{n}\sum_\beta\langle X_{L\beta}\rangle^2+\frac{B}{n}\sum_\beta\langle\delta X_{L\beta}\delta X_{L\beta}\rangle=0 .\end{aligned} \tag{31}$$

The local mean-square displacement fluctuation of a phonon system with harmonic time dependence [Eq. (26)] is given by

$$\langle\delta X_{L\alpha}^2\rangle=\frac{1}{2MN}\sum_{\vec{q}}\frac{1}{\omega(\vec{q})}\coth\frac{\omega(\vec{q})}{2k_BT} , \tag{32}$$

which is independent of α. Therefore [Eqs. (31) and (32)] the critical temperature is determined by

$$\frac{4dC-A}{B}=\langle\delta X_{L\alpha}^2\rangle=\frac{1}{2Mn}\sum_{\vec{q}}\frac{1}{\omega(\vec{q})}\times\coth\frac{\omega(\vec{q})}{2k_BT_c^{\text{quant}}} . \tag{33}$$

T_c^{quant} denotes the quantum-mechanical transition temperature. In contrast to this, the classical T_c^{cl} is given by

$$\frac{4dC-A}{B}=\langle\delta X_L^2\rangle_{\text{cl}}=\frac{k_BT_c^{\text{cl}}}{NM}\sum_{\vec{q}}\frac{1}{\omega^2(\vec{q})} . \tag{34}$$

From the inequality

$$\frac{1}{2k_B T\omega} \coth \frac{\omega}{2k_B T} \geq \frac{1}{\omega^2} , \tag{35}$$

we infer that

$$T_c^{\rm cl} \geq T_c^{\rm quant} . \tag{36}$$

For the quantum-mechanical displacive limit we obtain from Eqs. (16) and (32) for $d=3$

$$\frac{S_{\rm min}}{B} = \lim_{T\to 0} \frac{1}{2NM} \sum_{\vec{q}} \frac{1}{\omega(\vec{q})} \coth \frac{\omega(\vec{q})}{2k_B T} = \frac{1}{2NM} \sum_{\vec{q}} \frac{1}{\omega(\vec{q})} \bigg|_{T=0} = \frac{1}{2NM} \sum_{\vec{q}} \frac{1}{4\, C[3-F(\vec{q})]^{1/2}} \tag{37}$$

Thus, for any finite mass M and coupling constant C, the quantum-mechanical displacive limit occurs at a finite value of $4dC - A$.

Next, we consider the $S = 4dC - A$ dependence of T_c. Classical statistical mechanics predicts, according to Eq. (34), a linear relationship, namely,

$$T_c^{\rm cl} \sim S = 4dC - A . \tag{38}$$

To treat the quantum-mechanical case, we set

$$T = T_c^{\rm quant}(S) + [T - T_c^{\rm quant}(S)] = T_c^{\rm quant}(S) + \tau . \tag{39}$$

From Eqs. (31), (33), and (39) we find

$$M\omega^2(\vec{0}, S, \tau) = -S + \frac{B}{2Mn} \sum_{\vec{q}} \frac{1}{\omega(\vec{q})} \coth \frac{\omega(\vec{q})}{2k_B[T_c^{\rm quant}(S)+\tau]} , \tag{40}$$

so that at $\tau = 0$,

$$S = S_{\rm min} + \frac{B}{2MN} \sum_{\vec{q}} \frac{1}{\omega(\vec{q})} \left[\coth\left(\frac{\omega(\vec{q})}{2k_B T^{\rm quant}(S)}\right) - 1 \right] . \tag{41}$$

Thus, close to $T_c^{\rm quant}$ we obtain

$$S = S_{\rm min} + \frac{(T_c^{\rm quant})^2 M^{1/2} B}{C^{3/2}} \times \text{const} . \tag{42}$$

For $S \gg S_{\rm min}$, however, $T_c^{\rm quant}(S)$ approaches the classical behavior, as given by Eq. (38). The resulting S dependence of $T_c^{\rm quant}$ is shown in Fig. 1. For $S < S_{\rm min}$, we have no phase transition. At the quantum-mechanical displacive limit, $T_c^{\rm quant}$ vanishes and increases for $S > S_{\rm min}$, but small values of $S - S_{\rm min}$ according to the square-root law (42). $T_c^{\rm quant}(S)$ approaches the classical linear law (38) for $S \gg S_{\rm min}$.

To evaluate the critical exponents, we start from the integral equation determining $M\omega^2(\vec{q})$ and thus the static susceptibility. From Eqs. (31) and (32), we have

$$\chi_{\alpha\alpha}^{-1}(\vec{q}, \omega=0) = M\omega^2(\vec{q}) = A - 4C\, F(\vec{q}) + B\langle X_{L\alpha}\rangle^2 + \frac{B}{2NM} \sum_{\vec{q}} \frac{1}{\omega(\vec{q})} \coth \frac{\omega(\vec{q})}{2k_B T} . \tag{43}$$

For $T_c \neq 0$, the leading contribution to the q sum is obtained by expanding the hyperbolic cotangent with respect to small argument. Therefore, the exponents of the spherical model[26]

$$\alpha = \frac{d-4}{d-2}, \quad \beta = \tfrac{1}{2}, \quad \gamma = \frac{2}{d-2}, \quad \delta = \frac{d+2}{d-2}, \quad \eta = 0 , \tag{44}$$

for $2 < d < 4$ are obtained. For $d \leq 2$, there is no phase transition and for $d \geq 4$ mean-field exponents are found.

In the quantum-mechanical displacive limit ($T_c^{\rm quant} = 0$), care has to be taken as to the definition of some of the exponents. For instance, the q-dependent displacement-correlation function defined by

$$S(\vec{q}) = \frac{1}{2M\omega(\vec{q})} \coth \frac{\omega(\vec{q})}{2k_B T} \tag{45}$$

is no longer proportional to $\chi(\vec{q}, \omega=0)$ for $T = T_c^{\rm quant} = 0$. From Eqs. (43) and (45), we find for $T = T_c^{\rm quant} = 0$:

$$S(\vec{q}, \quad T = T_c^{\rm quant} = 0) \sim \frac{1}{2(2a^2 cq^2)^{1/2}} \sim \frac{1}{q} , \tag{46}$$

$$\chi(\vec{q}, \omega = 0, \quad T = T_c^{\rm quant} \sim 0) = \frac{1}{2a^2 C q^2} \sim \frac{1}{q^2} . \tag{47}$$

Thus, if we define for $T = T_c^{\rm quant} = 0$

$$S(\vec{q}) \sim q^{2-\eta}, \quad \chi(\vec{q}, 0) \sim q^{2-\bar{\eta}}, \tag{48}$$

we obtain

$$\eta = 1, \quad \bar{\eta} = 0. \tag{49}$$

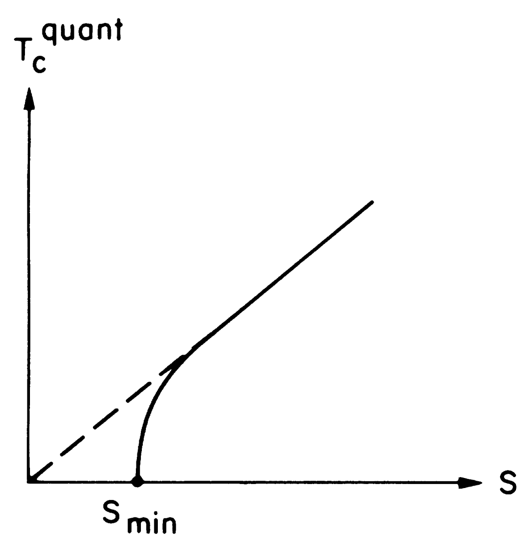

FIG. 1. $S = 12C - A$ dependence of the quantum-mechanical transition temperature in the limit $n = \infty$ at $d = 3$. The linear relationship is the classical result [Eq. (38)]. $S_{\rm min}$ denotes the quantum-mechanical displacive limit where the transition temperature vanishes.

Therefore, $\bar{\eta}$ has the classical value, whereas η, corresponding to the conventional definition of this exponent, is one. This discrepancy will be mirrored in the scaling laws.

To evaluate γ and δ, we write the frequency $\omega(\vec{q})$ for $M=1$ in the form

$$\omega^2(\vec{q}) = r + \varphi(\vec{q}), \quad \varphi(\vec{0}) = 0 \ . \tag{50}$$

Thus, the integral equation (43) determines r,

$$r = A - 4dC + BU^2 + \frac{B}{N}\sum_{\vec{q}} \frac{1}{[r+\varphi(\vec{q})]^{1/2}} \times\left[N_0\left(\frac{[r+\varphi(\vec{q})]^{1/2}}{k_B T}\right)+\frac{1}{2}\right]. \tag{51}$$

N_0 denotes the Bose function

$$N_0(X) = (e^X - 1)^{-1} \quad , \tag{52}$$

and U is the expectation value of any $X_{L\alpha}$ in the presence of a homogeneous field h. U is determined by the equation of state

$$U = h/r \quad , \tag{53}$$

which is essentially Eq. (4), simplified by virtue of Eqs. (18)–(20), (27), and (50). Equation (51) is cast into the form

$$r = A - 4dC + BU^2 T^{d-1}\,\Phi(r/T^2) + Z_0(r) \quad . \tag{54}$$

In Eqs. (B6) and (B8) of Appendix B, explicit expressions for Φ and Z_0 representing thermal and zero-point fluctuations in $\langle \delta X_{L\alpha}^2 \rangle$ are given.

Putting $T=0$, we find the critical exponent δ by inserting (53) into (54) and solving for $r(h)$. The result is

$$\delta = \frac{d+3}{d-1} \ \text{for}\ 1<d<3$$
$$\delta = 3 \quad \text{for}\ d \geq 3 \quad . \tag{55}$$

For $d<1$, there is no phase transition (see below) and for $d=3$ the exponent is 3, except for logarithmic corrections. Together with the value $\eta=1$ [Eq. (49)], the scaling relation[27]

$$\delta = (d+2-\eta)/(d-2+\eta) \tag{56}$$

is obviously violated. The Buckingham-Gunton inequality[27]

$$d\,\frac{\delta-1}{\delta+1} \geq 2-\eta \quad , \tag{57}$$

however is satisfied. Moreover, δ [Eq. (55)] differs from the value of the spherical model, because $\eta=1$. It is interesting to note that the mean-field domain for δ ranges down to $d=3$ in contrast to the usual case[16] of $d=4$. This is obviously due to the different "infrared" behavior of classical thermal fluctuations,

$$Z_{c1} \sim \int_0^1 dq\, q^{d-1}\,\frac{k_B T}{r+q^2} \quad , \tag{58}$$

and the quantum-mechanical zero-point fluctuations,

$$Z_0 \sim \int_0^1 dq\, q^{d-1}\,\frac{1}{(r+q^2)^{1/2}} \quad . \tag{59}$$

A similar observation was recently made by Holz and Medeiros,[28] who also found $\bar{\eta}$ (in our notation) remains unchanged to first order in $1/n$ for $d>3$ at the quantum-mechanical displacive limit.

The exponent γ is obtained from Eq. (54) by putting $U=0$. According to Eqs. (B6) and (B8) (see Appendix B), the following observations can be made: For $d \leq 1$, Z_0 diverges for $r \to 0$; thus, there is no phase transition. Again, this is different from the classical case for $T_c > 0$. There, the phase transition is suppressed by thermal fluctuations for $d \leq 2$. In the quantal case the zero-point fluctuations, being "weaker", shift the limit of dimensionality, where a phase transition might occur, down to one. For $1<d<3$, $r(T) \sim T^2 + \cdots$ [Eq. (54)]. Consequently, r/T^2 is a constant and so is the unknown function $\Phi(r/T^2)$. For $d=3$, the same is true, including, however, logarithmic corrections due to (B6). For $d>3$, we find $r \sim T^{d-1} + \cdots$. Here, $r/T^2 \sim T^{d-1}$, goes to zero for small T and $\Phi(r/T^2)$ can be replaced by its (finite) value for $r/T^2=0$. To summarize, we find

$$\gamma = 2, \quad 1<d\leq 3 \ ,$$
$$\gamma = d-1, \quad d>3 \ . \tag{60}$$

For the specific heat, the free energy and its derivatives with respect to T must be evaluated. This is most easily achieved by writing the Hamiltonian (2) in the form,

$$\mathcal{H} = \sum_{L,\alpha} \frac{P_{L\alpha}^2}{2M} + \frac{A}{2}\sum_{L,\alpha} X_{L\alpha}^2 + \frac{B}{2n}\sum_{L,\alpha\alpha'} \langle X_{L\alpha}^2 \rangle X_{L\alpha'}^2 - \frac{B}{4n}\sum_{L,\alpha\alpha'} \langle X_{L\alpha}^2\rangle\langle X_{L\alpha}^2\rangle - C\sum_{L,L',\alpha} X_{L\alpha}X_{L'\alpha'} + V \ , \tag{61}$$

where

$$V = \frac{B}{4n}\sum_{L,\alpha\alpha'} X_{L\alpha'}^2 X_{L\alpha}^2 - \frac{B}{2n}\sum_{L\alpha\alpha'} \langle X_{L\alpha}^2\rangle X_{L\alpha'}^2 + \frac{B}{4n}\sum_{L\alpha\alpha'} \langle X_{L\alpha}^2\rangle\langle X_{L\alpha'}^2\rangle \ . \tag{62}$$

It is easy to verify that (61) is the appropriate effective Hamiltonian for the large n limit, because the contributions of V to the partition function vanishes for $n\to\infty$. By using Eqs. (27) and (50) and the usual expression for the free energy of a harmonic phonon system one ends up with

$$F = \frac{1}{N}\,k_B T\sum_{\vec{q}} \ln\left(2\sinh\frac{\omega(\vec{q})}{2k_B T}\right) - \frac{1}{4B}\,(r-r_0)^2 \tag{63}$$

for the free energy per particle and per component for $n=\infty$. Here

$$r_0 = A - 4dC \, . \tag{64}$$

The exponent of the specific heat,

$$C_V = -T \frac{\partial^2 F}{\partial T^2} \, , \tag{65}$$

can again be defined in two ways. Because $T_c^{\text{quant}} = 0$ at the displacive limit, the factor T in front of the second derivative (usually replaced by T_c) weakens a possible singularity of C_V (for $T \to T_c^{\text{quant}} = 0$). We thus define

$$C_V \sim T^{-\bar{\alpha}}$$
$$C_V/T \sim T^{-\alpha} \, , \tag{66}$$

where

$$\alpha = \bar{\alpha} + 1 \, . \tag{67}$$

α corresponds to the usual specific-heat exponent. Explicit differentiation of (63) yields, by invoking Eq. (B7) (Appendix B),

$$c_V = T^d \int dX \, X^{d-1} \frac{e(R+X^2)^{1/2}}{[e(R+X^2)^{1/2} - 1]^2} \left(R + X^2 - \frac{1}{2T} \frac{\partial r}{\partial T} \right) , \tag{68}$$

where

$$R = r/T^2 \, . \tag{69}$$

Using similar arguments as for γ, we find

$$\bar{\alpha} = -d \, ,$$
$$\alpha = 1 - d \, , \tag{70}$$

except for logarithmic corrections for $d=3$.

Finally, we turn to the correlation length ξ, which might be defined by

$$\xi^2 = -\left(\frac{1}{\chi(\vec{q})} \frac{d^2 \chi(\vec{q})}{dq^2} \right)_{\vec{q}=0} \, , \tag{71}$$

where $\chi(\vec{q})$ is given by Eqs. (43) and (50). After some algebra we conclude, using the previous result for γ [Eq. (60)], that

$$\nu = \gamma/2 \, , \tag{72}$$

which is in agreement with the scaling law,[27]

$$\gamma = (2 - \bar{\eta}) \, \nu \, . \tag{73}$$

Finally, we remark that the scaling relation,[27]

$$\delta = \frac{2 - \alpha + \gamma}{2 - \alpha - \gamma} \, , \tag{74}$$

is fulfilled.

IV. SUMMARY AND CONCLUSIONS

We have explored the influence of zero-point oscillations in an n-component vector model for structural phase transitions.

An important result is that this quantum effect can suppress the occurrence of a phase transition for $n=1$, 2 and $n=\infty$ and all dimensionalities d. The fact that there is no ferroelectric phase transition in $SrTiO_3$ at normal pressure may be a prominent example for this quantum effect. In fact, the dielectric constant is found to increase with decreasing temperature as high as 10^4 in the liquid-He temperature range.[29,30] However, deviation from the Curie-Weiss behavior is manifest below 60 K, being interpreted as due to zero-point oscillation.[31,32] Concerning the applicability of our results, which are valid for $n=1$, 2 and $n=\infty$, to $SrTiO_3$ one has to bear in mind that the critical behavior of a system with Hamiltonian (1) may depend on the stress conditions. In fact, Bruce and Aharony[6] have shown that the critical behavior might be of Ising, $X-Y$ or Heisenberg type.

The suppression of a phase transition due to zero-point oscillations was found to be of particular relevance for systems having model parameters close to the classical displacive limit.[20-22] Here, a phase transition can be suppressed if the mass of the particles is sufficiently small. The classical displacive limit has been replaced by the quantum-mechanical analog. A common feature of these limits is, at least for $n=\infty$, that they represent an isolated point in the space of the model parameters, having different exponents.

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APPENDIX A

For classical systems, inequalities like Eq. (11) were established by Guerra, Rosen, and Simon[24] for $n=1$, and by Dunlop and Newman[25] for $n=2$. This inequality represents an extension of the second Griffiths-Kelly-Sherman inequality to continuous variables.

The proof rest upon the fact that correlation functions like,

$$\langle X_{L\alpha}^3 \rangle = \frac{1}{Z} \int \prod_{p=1}^{N} \prod_{\alpha=1}^{n} dX_{p\alpha} X_{L\alpha}^3 \, \rho \, (\vec{X}_1 , \ldots , \vec{X}_N), \tag{A1}$$

are integrals over a ferromagnetic measure ρ, which in this case is the classical distribution function $e^{-\beta V}$.

Extension of the inequality to quantum mechanics is most easily done by replacing the trace by an integral over a suitable ferromagnetic measure.

To derive this measure we first consider an anharmonic oscillator with Hamiltonian

$$\mathcal{H} = \vec{P}^2/2M + V(\vec{X}) = T + V \, , \tag{A2}$$

where

$$V(\vec{X}) = \tfrac{1}{2}A\vec{X}^2 + (B/4n)\vec{X}^4 \, , \tag{A3}$$

$$\vec{X} = (X_1 \, , \, \cdots, \, X_\alpha \cdots, \, X_n) \, . \tag{A4}$$

Next we introduce the X representation of the density matrix,[33]

$$\rho\,(\vec{X}_0, \, \vec{X}_r) = \langle \vec{X}_0 \mid \rho \mid \vec{X}_r \rangle \quad . \tag{A5}$$

Using the Trotter formula,[34]

$$e^{-\beta\mathcal{H}} = \lim_{m\to\infty} \left[\exp\left(-\frac{\beta T}{m}\right)\exp\left(-\frac{\beta V}{m}\right)\right]^m \, , \tag{A6}$$

we may rewrite (A5) in the form

$$\rho\,(\vec{X}_0, \, \vec{X}_r) = \lim_{m\to\infty} \langle \vec{X}_0 \mid \left[\exp\left(-\frac{\beta T}{m}\right)\exp\left(-\frac{\beta V}{m}\right)\right]^m \mid \vec{X}_r \rangle$$

$$= \lim_{m\to\infty} \int \prod_{i=1}^{m-1} d^n X_i \, \rho_m\,(\vec{X}_0 \, , \, \ldots \, , \, \vec{X}_r) \, , \tag{A7}$$

where

$$\rho_m\,(\vec{X}_0, \, \cdots, \, \vec{X}_r) = \exp\left[-\beta V(\vec{X}_r)\right] \rho_0\,(\vec{X}_{m-1} - \vec{X}_r) \times \prod_{i=1}^{m-1} \exp\left[\frac{\beta V(\vec{X}_i)}{m}\right] \prod_{i=1}^{m=1} \rho_0\,(\vec{X}_{i-1} - \vec{X}_i) \, , \tag{A8}$$

$$\rho_0\,(\vec{X}_{i=1} - \vec{X}_i) = C_n \left(\frac{2Mm}{\beta}\right)^{n/2} \times \exp\left(-\frac{Mm}{2\beta}\,(\vec{X}_{i-1}^2 + \vec{X}_i)^2\right) \exp\left(\frac{Mm}{\beta}\,\vec{X}_{i-1}\,\vec{X}_i\right) \tag{A9}$$

$$C_n^{-1} = \int d^n X \, \exp(-\vec{X}^2) \quad . \tag{A10}$$

On this basis, correlation functions like (A1) can be expressed as

$$\langle \vec{X}^3 \rangle = \lim_{m\to\infty} \frac{1}{Z} \int \prod_{i=0}^{m-1} d^n X_i \, X_{0\alpha}^3 \, \rho_m \times (\vec{X}_0, \, \ldots, \, \vec{X}_{m-1}, \, \vec{X}_0) \, , \tag{A11}$$

where

$$Z = \lim_{m\to\infty} \int \prod_{i=0}^{m-1} d^n X_i \, \rho_m\,(\vec{X}_0 \, , \cdots, \, \vec{X}_{m-1}, \, \vec{X}_0). \tag{A12}$$

Obviously, (A11) is again an integral with a ferromagnetic measure. Thus the noncommutative properties of kinetic and potential energy lead to the following modifications with respect to the classical distribution functions: (i) ρ_m describes m-identical n-component oscillators with a ferromagnetic nearest-neighbor coupling. (ii) The single-particle measure of each oscillator is modified.

Next we consider N such oscillators with a ferromagnetic coupling. The Hamiltonian reads [see Eq. (2)],

$$\mathcal{H} = \sum_{l=1}^{N} \left\{\frac{P_l^2}{2M} + V(\vec{X}_l)\right\} - C \sum_{l,\, l'=1}^{N} \sum_{\alpha=1}^{n} X_{l\alpha} \, X_{l'\alpha} . \tag{A13}$$

Defining

$$\vec{X}_{il} = \{X_{il1}, \, \cdots, X_{il\alpha}, \, X_{iln}\} \, ,$$

where

$$i = 0, \, \cdots, \, m, \; l = 1, \, \cdots, \, N \tag{A14}$$

we obtain in analogy to Eq. (A8)

$$\rho_m\,(\{X_{i\alpha}\}) = C_n^{mN}\left(\frac{2Mm}{\beta}\right)^{mNn/2} \times\exp\left(-\frac{Mm}{2\beta}\sum_{l=1}^{N}(\vec{X}_{0l}^2 + \vec{X}_{ml}^2)\right) \times\exp\left(-\frac{Mm}{\beta}\sum_{i=l}^{m=1}\sum_{l=1}^{N}\vec{X}_{il}^2\right)\exp\left(-\frac{\beta}{m}\sum_{i=1}^{m}\sum_{l=1}^{N}V(\vec{X}_{il})\right) \times\exp\left(\frac{Mm}{\beta}\sum_{i=1}^{m}\sum_{l=1}^{N}\vec{X}_{i-1,\,l}\vec{X}_{i,\,l}\right) \times\exp\left(\frac{\beta}{m}\,C\sum_{i=1}^{m}\sum_{l,\,l'=1}^{N}\sum_{\alpha=1}^{n}X_{il\alpha}\,X_{il'\alpha}\right) . \tag{A15}$$

The last two terms again describe ferromagnetic couplings. Consequently, the measure ρ_m is again ferromagnetic. The partition function is then given by

$$Z = \mathrm{Tr}\rho^{-\beta\mathcal{H}} = \lim_{m\to\infty} Z_m \, , \tag{A16}$$

where

$$Z_m = \int \rho_m\,(\{\vec{X}_{il}\}) \prod_{i=0}^{m}\prod_{l=1}^{N} d^n X_{il} \, , \tag{A17}$$

and a typical correlation function reads

$$\langle X_{l\beta}^2 X_{l'\alpha} \rangle = \frac{1}{Z}\lim_{m\to\infty}\int \rho_m\,(\{\vec{X}_{il}\})\,X_{0l\beta}^2\,X_{0l'\alpha}\prod_{i=0}^{m}\prod_{l=1}^{N} d^n X_{il} \, . \tag{A18}$$

To summarize, we have shown how the trace is transformed into an integral over a ferromagnetic measure. Therefore,[23–25] all classical inequalities for systems with continuous variables and ferromagnetic coupling also hold in quantum mechanics for lattice-dynamical systems.

APPENDIX B

We have to calculate

$$\langle \delta X^2_{L\alpha}\rangle = \frac{B}{N}\sum_{\vec{q}} \frac{1}{[r+\varphi(\vec{q})]^{1/2}} \times\left[N_0\left(\frac{[r+\varphi(\vec{q})]^{1/2}}{k_B T}\right)+\frac{1}{2}\right] . \quad (B1)$$

For an infinite system the $\vec{q}$ sum is converted to an integral. For a cubic system in d dimensions it is sufficient to approximate $\varphi(\vec{q})$ by its small q behavior

$$\varphi(\vec{q}) \sim q^2 \quad , \quad (B2)$$

and to integrate over a sphere of radius Λ. Neglecting the uninteresting constants we have to deal with two integrals of the form

$$\langle \delta X^2_{L\alpha}\rangle \sim Z_{\text{th}}(r,T)+Z_0(r) \quad , \quad (B3)$$

where

$$Z_{\text{th}}(r,T) = \int_0^1 dq\, q^{d-1}\, 1\, \frac{1}{r+q^2)^{1/2}} N_0\left(\frac{(r+q^2)^{1/2}}{k_B T}\right) , \quad (B4)$$

$$Z_0(r) = \frac{1}{2}\int_0^1 dq \frac{q^{d-1}}{(r+q^2)^{1/2}} \quad . \quad (B5)$$

Z_{th} represents the effects of the thermal, and Z_0 of the zero-point oscillations in $\langle \delta X^2_{L\alpha}\rangle$. For low temperatures the integration in (B4) can be extended to infinity. Z_0 can be evaluated explicitly. The result depends on the dimensionality d. To lowest order in r we find

$$\begin{aligned} &d=1, \quad Z_0=a-b\ln r \\ &1<d<3, \quad Z_0=a-br-cr^{(d-1)/2}+\cdots \\ &d=3, \quad Z_0=a-br+cr\ln r \\ &d>3, \quad Z_0=a-br+\cdots \quad . \end{aligned} \quad (B6)$$

Higher powers in r than those given here would not alter the critical exponents calculated in Sec. III. Z_{th} cannot be given in closed form. By means of the transformation

$$q=TX, \quad r=RT^2 \quad , \quad (B7)$$

which is well defined for $T\neq 0$ (for $T=0$, Z_{th} vanishes), we find

$$Z_{\text{th}}(r,T)=T^{d-1}\,\Phi(R) \quad , \quad (B8)$$

where

$$\Phi(R)=\int_0^\infty dX \frac{X^{d-1}}{(R+X^2)^{1/2}} N_0\,(R+X^2)^{1/2} \quad . \quad (B9)$$

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