Classical displacive limit of an n-component model for structural phase transitions

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The static critical behavior of an n-component model at the displacive limit is investigated by means of classical mechanics. In the large-n limit, critical exponents and crossover behavior are found by explicit calculation, whereas renormalization-group and scaling relations are used to treat the case of general n exactly for arbitrary dimension. The exponents at the displacive limit, i.e., for $T_c = 0$, are classical for $d > 2$. They are independent of n and differ from those of $T_c > 0$ for $d < 4$.

I. INTRODUCTION

We consider the usual n-vector Hamiltonian

$$H=\sum_{l\alpha}\frac{p_{l\alpha}^2}{2M}+\tfrac{1}{2}A\sum_{l\alpha}x_{l\alpha}^2+\frac{B}{4n}\sum_{l\alpha\alpha'}x_{l\alpha}^2x_{l\alpha'}^2-\tfrac{1}{2}C\sum_{ll'\alpha}x_{l\alpha}x_{l'\alpha}. \quad (1.1)$$

This form has been used as a model for structural phase transitions.[1,2] In this framework, $x_{l\alpha}$ and $p_{l\alpha}$ denote the α component of displacement and momentum ($1 \leq \alpha \leq n$) of the particle at lattice site $\vec{R}_l$, respectively. The sum over l and l' in the last term is restricted to nearest neighbors, for simplicity. Similar Hamiltonians as (1.1) can also describe transitions in classical magnetic systems. For this purpose the kinetic energy is usually omitted and $x_{l\alpha}$ is interpreted as the αth component of a continuous spin vector attached to site l. Most of the recent renormalization-group work[3-5] has in fact been performed with the potential-energy part of (1.1). More specifically, one uses the corresponding expression in $\vec{q}$ space, taking into account only a small-$\vec{q}$ expansion of the "dynamical matrix" [see our Eq. (3.5)]. For the magnetic case, A is usually chosen to be negative. Thus the one-particle distribution function

$$P(\vec{x}_l)=\exp\left\{-\left[\beta\left(\tfrac{1}{2}A\sum_\alpha x_{l\alpha}^2+\tfrac{1}{4}B\left(\sum_\alpha x_{l\alpha}^2\right)^2\right]\right\} \quad (1.2)$$

is a good approximation to a classical spin system, where

$$\sum_\alpha x_{l\alpha}^2 = s^2 \quad (1.3)$$

(i.e., the spin vectors have fixed length s). In fact, if $A\to-\infty$, $B\to+\infty$, $A/B=$ const, (1.2) reduces to $\delta(\sum_\alpha x_{l\alpha}^2 - s^2)$. In the case of structural transitions, both regimes $A<0$ (order-disorder transitions) and $A>0$ (displacive transitions) are of interest.[6] In the displacive domain considered here the existence of an ordered phase with nonvanishing order parameter $\langle x_{l\alpha}\rangle$ depends on the relative magnitude of A and C. (The latter is supposed to be positive.) At $T=0$ the ordered phase is more stable for a classical system if

$$r_0 \equiv A - zC < 0, \quad (1.4)$$

z being the number of nearest neighbors.

In the limit of n going to infinity the static and the dynamic properties of (1.1) can be evaluated exactly.[1] A phase transition occurs for dimensionality $d>2$, provided that (1.4) is valid, and the static exponents agree with those of the spherical model[7] and with those of a model with $n=1$ but with the quartic term in (1.1) replaced by a long-range anharmonic interaction.[8] Moreover, the existence of a phase transition has been proved rigorously[9] for $n=1$ for the full order-disorder regime and for some part of the displacive regime.

According to the principle of universality, the static critical exponents should be the same all over the domain of those A and C values which allow for a transition, as long as n and d are fixed. This need not be true for the so-called displacive limit, i.e., where $T_c=0$. We expect this to occur in classical mechanics for $r_0=0$. This is an "isolated point" in the parameter space of A, B, and C. It is the purpose of this work to evaluate critical exponents for this limit and to calculate the crossover behavior which is expected, since these exponents differ from the ones valid away from the displacive limit.

In Sec. II the calculations are done explicitly for $n\to\infty$, while Sec. III deals with arbitrary n by means of renormalization-group techniques. Unlike the usual situation with $T_c>0$, where exponents can only be obtained in powers of $\epsilon=4-d$ the displacive limit allows for some exact results for arbitrary n and d. This is the (formally) interesting aspect of the classical displacive limit.[10,11] In reality one may argue that if the critical temperature is zero, quantum effects are no longer negligible. The quantum-mechanical displacive limit, where zero-point fluctuations dominate the critical behavior, will be treated in a further publication,[12] where the physical relevance for real systems will also be discussed.

II. LARGE-n LIMIT

In order to have a guide for general n it is useful to study the limit $n \to \infty$ which can be treated exactly. Here the static structure factor

$$S_\alpha(\vec{q}) = \sum_l \langle x_{l\alpha} x_{0\alpha} \rangle \, e^{i\vec{q}\cdot\vec{R}_l} \tag{2.1}$$

is given by

$$S_\alpha(\vec{q}) = k_B T \chi(\vec{q}) = k_B T / \omega^2(\vec{q}). \tag{2.2}$$

$\chi(\vec{q})$ is the static susceptibility (independent of α for $T > T_c = 0$), and the frequency $\omega(\vec{q})$ is the solution of the self-consistent phonon equation

$$\omega^2(\vec{q}) = r_0 + g(\vec{q}) + \frac{B k_B T}{N} \sum_{\vec{q}'} \frac{1}{\omega^2(\vec{q}')} , \tag{2.3}$$

with

$$g(\vec{q}) = C\left(\sum_{\mathrm{ln},N} e^{i\vec{q}\cdot\vec{R}_l}\right) - z = b^2\vec{q}^2 + O(\vec{q}^4). \tag{2.4}$$

For cubic lattices it is sufficient to take the term $b^2\vec{q}^2$ in order to determine the critical behavior. For small $\vec{q}$ the solution of (2.3) is of the form

$$\omega^2(\vec{q}) = r + b^2\vec{q}^2, \tag{2.5}$$

r being determined by

$$r = r_0 + \frac{B k_B T}{N} \sum_{\vec{q}} \frac{1}{r + b^2\vec{q}^2} . \tag{2.6}$$

For an infinite system the $\vec{q}$ sum is replaced by an integral over a spherical Brillouin zone with some cutoff radius Λ. At the displacive limit ($r_0 = 0$) we find

$$r = T\phi(r), \tag{2.7}$$

with

$$\phi(r) \sim \int_0^\Lambda dq\, q^{d-1} \frac{1}{r+q^2} = \begin{cases} a r^{d/2-1} + \cdots & \text{for } d < 2, \\ c - a \ln r + \cdots & \text{for } d = 2, \\ c - a r^{d/2} - 1 + \cdots & \text{for } 2 < d < 4, \\ c + e r - a r \ln r + \cdots & \text{for } d = 4, \\ c + e r + \cdots & \text{for } d > 4. \end{cases} \tag{2.8}$$

The (cutoff dependent) values of the constants are irrelevant for the critical behavior. Moreover Eqs. (2.8) only show the leading powers of r. We find

$$\chi(\vec{q} = \vec{0}) \sim (T - T_c)^{-\gamma} = T^{-\gamma}, \tag{2.9}$$

with

$$\gamma = \begin{cases} 2/(4-d) & \text{for } d < 2, \\ 1 & \text{for } d > 2. \end{cases} \tag{2.10a}$$

In two dimensions $\gamma = 1$. However, there are logarithmic corrections to the form (2.9).

The values (2.10a) of γ do not agree with the usual ones for $r_0 < 0$, which are

$$\gamma = \begin{cases} 2/(2-d) & \text{for } d < 2, \\ 2/(d-2) & \text{for } 2 < d < 4, \\ 1 & \text{for } d > 4. \end{cases} \tag{2.10b}$$

(For $d < 2$ there is no ordered phase for any finite temperature in the $n \to \infty$ limit, but for $r_0 < 0$ the susceptibility χ diverges for $T \to T_c = 0$, see the end of this section.) In the displacive limit γ takes the molecular-field value for $d > 2$ instead of $d > 4$ as usual. The border between mean-field and nonclassical behavior ($d = 2$ here) has logarithmic corrections as is usually the case for $d = 4$.

From (2.5) it immediately follows that $\eta = 0$. The correlation length is best defined by

$$\xi^2 = -\left(\frac{dS_\alpha(\vec{q})}{d\vec{q}^2} \frac{1}{S_\alpha(\vec{q})}\right)_{\vec{q}=\vec{0}} , \tag{2.11}$$

since S_α itself vanishes at $T = 0$. This yields

$$\xi \sim T^{-\nu}, \quad \text{with } \nu = \tfrac{1}{2}\gamma. \tag{2.12}$$

The displacement M_α induced by an external field H_α at $T = T_c = 0$ is easily calculated from the equation of state

$$M_\alpha r_0 + \frac{B}{n}\left(M_\alpha^3 + k_B T M_\alpha \sum_{\vec{q}} \frac{1}{\omega^2(\vec{q}, H_\alpha)}\right) = H_\alpha. \tag{2.13}$$

The result is

$$M_\alpha \propto H_\alpha^{1/\delta}, \tag{2.14}$$

with $\delta = 3$ for all dimensions. The specific heat is calculated in the same way as for the spherical model.[7] The partition function can be evaluated by noting that

$$\exp\left[-\beta\frac{B}{4n}\sum_l\left(\sum_\alpha x_{l\alpha}^2\right)^2\right] = (2\Pi)^{-N/2}\int\prod_{l=1}^N ds_l \exp\left[-\frac{1}{2}\sum_l s_l^2 + i\sqrt{2}\sum_l s_l\left(\frac{\beta B}{4n}\right)^{1/2}\sum_\alpha x_{l\alpha}^2\right]. \tag{2.15}$$

This formula allows one to use the steepest-descent method in the limit $n \to \infty$ as for the spherical model.[7] The free energy per particle and per component of the order parameter is

$$\frac{F}{nN} = -\frac{(r-r_0)^2}{4B} + \frac{k_B T}{2N} \sum_{\vec{q}} \ln(r + \vec{q}^{\,2}). \tag{2.16}$$

Using relations (2.3), (2.5), and (2.6) this yields for the specific heat

$$C_v(T) = -T\left(\frac{\partial^2 F}{\partial T^2}\right) = -\frac{r-r_0}{2B}\frac{\partial r}{\partial T}. \tag{2.17}$$

At the displacive limit

$$C_v \sim T^{2\gamma-1} \sim T^{-\bar{\alpha}}, \tag{2.18}$$

with

$$\bar{\alpha} = \begin{cases} -d/(4-d) & \text{for } d<2, \\ -1 & \text{for } d>2. \end{cases} \tag{2.19}$$

In order to check scaling relations involving the specific-heat exponent α one should choose

$$\alpha = \bar{\alpha} + 1, \tag{2.20}$$

because at $T = T_c = 0$ the factor T in the definition (2.17), which is usually replaced by T_c, weakens a possibly singular behavior of C by one power of $T = T - T_c$. Equations (2.10), (2.12), (2.19), and (2.20) show that the exponent relations

$$\gamma = (2-\eta)\nu$$

and (2.21)

$$\delta = (2-\alpha+\gamma)/(2-\alpha-\gamma)$$

are fulfilled. Those relations which involve the dimension are violated. In fact we find

$$\delta = (D+2)/(D-2) \tag{2.22}$$

and

$$2-\alpha = D\nu, \tag{2.23}$$

with $D = 4$, i.e., the system behaves in this respect as if it were four dimensional.

Finally, we calculate the crossover form of $\chi(r_0, \tau)$ as well as the crossover exponent ϕ describing the deviation from behavior (2.9) and (2.10) for nonvanishing negative r_0. For $2 < d < 4$ we find, using (2.6) and (2.8),

$$r = r_0 + T(c - ar^s), \quad s = \tfrac{1}{2}d - 1 > 0. \tag{2.24}$$

The critical temperature T_c is determined by $r = 0$, thus

$$r_0 + T_c c = 0. \tag{2.25}$$

With the help of this condition (2.24) is brought into the form

$$\frac{r}{\tau} = c + \frac{r_0}{c\tau^{1-s}}\left(\frac{r}{\tau}\right)^s - A\left(\frac{r}{\tau}\right)^s \tau^s, \tag{2.26}$$

with $\tau = T - T_c(r_0)$. The last term can be neglected in the critical region, where τ is small. Thus (2.26) implies

$$r = \tau g(r_0/\tau^{\phi}). \tag{2.27}$$

Here $g(x)$ is the crossover function, and the crossover exponent ϕ is given by

$$\phi = 1 - s = \tfrac{1}{2}(4-d). \tag{2.28}$$

The susceptibility χ takes the form

$$\chi(r_0, \tau) = \tau^{-1}(g(r_0/\tau^{\phi}))^{-1}. \tag{2.29}$$

For $d < 2$, Eq. (2.6) yields

$$r = r_0 + aTr^s, \quad s = \tfrac{1}{2}d - 1 < 0. \tag{2.30}$$

For these dimensions the critical temperature is $T_c = 0$; r goes to zero and χ diverges for $T \to 0$, provided that $r_0 \leq 0$. However, the critical exponents again differ for $r_0 \neq 0$ and $r_0 = 0$. Equation (2.30) is written

$$r/\tau^{\gamma_0} = r_0/\tau^{\gamma_0} + a(r/\tau^{\gamma_0})^s, \tag{2.31}$$

with

$$\gamma_0 = 1/(1-s) = 2/(4-d), \tag{2.32}$$

as found in (2.10). Thus

$$r = \tau^{\gamma_0} g(r_0/\tau^{\phi}), \tag{2.33}$$

with

$$\phi = \gamma_0 = 2/(4-d). \tag{2.34}$$

For small x the shape function $g(x)$ tends to a constant, which produces the behavior (2.9) and (2.10) for χ, whereas for large x the leading term is

$$g(x) \xrightarrow[x\to\infty]{} x^{1/s}. \tag{2.35}$$

Thus, away from the displacive limit, we end up with

$$r(\tau) \sim \tau^{\gamma_0(1-1/s)} = \tau^{-1/s} \tag{2.36}$$

and therefore

$$\gamma = -1/s = 2/(2-d), \tag{2.37}$$

as shown in Eq. (2.10b).

III. RENORMALIZATION-GROUP TREATMENT FOR GENERAL n

Recently, some rigoruous results concerning the displacive limit of (1.1) for $n = 1$ have been derived. Morf and Thomas[10] calculated the partition function and static susceptibility of a linear chain with the help of the transfer-operator technique. They found

$$\nu=\tfrac{1}{3},\quad \gamma=\tfrac{2}{3},\quad \alpha=\tfrac{2}{3},\quad \bar{\alpha}=-\tfrac{1}{3}, \tag{3.1}$$

as well as a crossover behavior of the form

$$\chi(r_0,\tau)=\tau^{-\gamma}g(r_0/\tau^{\phi}), \tag{3.2}$$

with

$$\phi=\tfrac{2}{3}. \tag{3.3}$$

By means of Green's function methods, Wiesner[11] found for $n=1$,

$$\phi=\begin{cases}\frac{2}{3} & \text{for } d=1,\\ 1 & \text{for } d\geq 2.\end{cases} \tag{3.4}$$

This result, valid for $n=1$, agrees with the large-n limit studied in Sec. II for $d\leq 2$, even though Wiesner[11] used a different definition of the crossover exponent. In order to treat arbitrary n we apply Wilson's renormalization-group approach to Hamiltonian (1.1). For this purpose the latter is, as usual, transformed into

$$H=\tfrac{1}{2}\sum_{\alpha}\int d^dq\,(r+q^2)x_\alpha(\vec{q})x_\alpha(-\vec{q})+\tfrac{1}{4}u\iint d^dq_1\cdots d^dq_4\,\delta\Big(\sum_{i=1}^{4}\vec{q}_i\Big)\sum_{\alpha\alpha'}x_\alpha(\vec{q}_1)x_\alpha(\vec{q}_2)x_{\alpha'}(\vec{q}_3)x_{\alpha'}(\vec{q}_4). \tag{3.5}$$

Many authors[3-5] have derived recursion relations for the parameters r and u under the effect of a renormalization-group transformation. Such a transformation is generated by eliminating the degrees of freedom with $|\vec{q}|>1/L$ and looking for a new, effective Hamiltonian involving parameters r' and u'. Our analysis differs from all this work in one respect: since we are interested in $T_c=0$ we cannot absorb the quantity $\beta=(k_BT)^{-1}$ showing up in the partition function, into the parameters of the Hamiltonian. Instead we have to keep track of all factors T explicitly. Consequently, the effective four-point coupling becomes small as $T\to 0$, and the ordering of the graphs is done with respect to powers of T. For example, expectation values of the form

$$\langle x_\alpha(\vec{q})x_{\alpha'}(\vec{q}')\rangle=\delta_{\alpha\alpha'}\delta(\vec{q}+\vec{q}')k_BT/(r+q^2) \tag{3.6}$$

(evaluated in the "Gaussian" approximation), which arise in the perturbative treatment of renormalization are linear in T. Therefore the explicit recursion relations—Eqs. (6.18) and (6.19) of Ref. 5—read

$$r'=L^2[r+4(n+1)uTA_1(r,L)+\cdots], \tag{3.7}$$

$$u'=L^{\epsilon}[u-4(n+8)u^2TA_2(r,L)+\cdots], \tag{3.8}$$

with

$$A_1=\int_{1/L}^{1}\frac{dq}{r+q^2} \tag{3.9}$$

and

$$A_2=\int_{1/L}^{1}\frac{dq}{(r+q^2)^2}\ . \tag{3.10}$$

Equations (3.7) and (3.8) are correct up to order ϵ ($\epsilon=4-d$), the dots pointing to higher-order terms $\sim\epsilon^2$, ϵ^3, etc. In our context, however, the important fact is that higher-order contributions also involve higher powers of T, since diagrams of higher order in the perturbation expansion of the partition function with respect to small u also involve higher powers of the propagator (3.6). Therefore we find for the displacive limit, $T_c=0$, a fixed point of (3.7) and (3.8) which is correct for arbitrary dimension, namely,

$$r^*=u^*=0. \tag{3.11}$$

Although these are the values which r and u assume at the Gaussian fix point, the exponents need not be classical, since, close to the fix point the recursion relations (linearized with respect to $\delta r=r-r^*$ and $\delta u=u-u^*$) have two relevant variables for $d<4$ (i.e., $\epsilon>0$):

$$\begin{pmatrix}\delta r'\\ \delta u'\end{pmatrix}=\begin{pmatrix}L^2 & 0\\ 0 & L^{\epsilon}\end{pmatrix}\begin{pmatrix}\delta r\\ \delta u\end{pmatrix}, \tag{3.12}$$

pointing to a crossover away from the fixed point (3.11), which would indeed take place if T_c were greater than zero. According to the general rules of renormalization-group theory[3-5] we first determine the exponent ν of the correlation length, which is given by the largest eigenvalue (of the form L^s) of (3.12):

$$\nu=\frac{\ln L}{\ln L^s}\begin{cases}1/\epsilon=1/(4-d) & \text{for } d<2\ \ (\epsilon>2),\\ \frac{1}{2} & \text{for } d>2\ \ (\epsilon<2).\end{cases} \tag{3.13}$$

This again shows that the borderline between mean-field and nonclassical behavior lies at $d=2$. Next, the crossover exponent is given by the ratio of the "weaker" and the "stronger" exponents in (3.12):

$$\phi=\begin{cases}2/\epsilon=2/(4-d) & \text{for } d<2,\\ \frac{1}{2}\epsilon=\frac{1}{2}(4-d) & \text{for } d>2.\end{cases} \tag{3.14}$$

For $d>4$, ϕ is negative: the Gaussian fixpoint is stable for all T_c, as is wellknown. The exponent δ need not be determined by renormalization theory, since at $T=T_c=0$ there are no more thermal fluctuations. Landau theory is exact and therefore $\delta=3$ for all d and n. From this and the scaling relations (2.21) we again obtain

$$\alpha = \bar{\alpha} + 1 = \begin{cases} 1 - d/(4-d) & \text{for } d < 2, \\ 0 & \text{for } d > 2. \end{cases} \tag{3.15}$$

All these results confirm that the static exponents are independent of n in the classical displacive limit. It is also interesting to compare the different borderlines between molecular-field and true critical behavior: (a) For $T_c > 0$, i.e., away from the displacive limit, thermal fluctuations cause deviations from Landau theory for $d < 4$. (b) At the quantum-mechanical displacive limit there are only zero-point fluctuations.[12,13] Their "infrared" behavior is less singular than that of thermal fluctuations; there is some kind of a borderline at $d = 3$ (which is reflected, for example, in δ), at least for $n \to \infty$, although some exponents take nonclassical values for all dimensions. (c) At the classical displacive limit, thermal fluctuations are weakened by factors of T [see, for example, our Eq. (3.6), and the integral equation (2.6)]. Thus the critical behavior is classical for $d > 2$.

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We have benefitted from conversations with H. Thomas and R. Morf. While writing this work we learned that R. Oppermann[13] came to similar conclusions concerning the classical displacive limit of the n-vector model.

Note added in proof. The renormalization-group arguments can be presented in a slightly different way, which makes the determination of ν and ϕ more transparent. By scaling the field variables in (3.5) by $T^{1/2}$ the inverse temperature in the partition function is, as usual, incorporated in the Hamiltonian. The quartic coupling parameter u is then proportional to T. The recursion relations have no explicit factors of T, but the eigenvalues at the Gaussian fixed point are the same as in (3.12). At the displacive limits, the renormalization procedure starts from $r = 0$, thus both scaling fields (δr and a linear combination of δu and δr) are proportional to T. The correlation length then scales as

$$\xi = L\xi(L^2 aT, L^{\epsilon} bT),$$

which immediately yields (3.13) for ν. Away from the displacive limit the starting value r is different from zero which leads to scaling fields of the form $aT + \delta$. The scaling properties of ξ then yield the crossover exponent as in (3.14). It should again be emphasized that the quantity τ showing up in crossover form like (2.29) is the difference between T and $T_c(r_0)$.

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