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Peculiarities of the $O(n)$ model for $n < 1$

P. D. Gujrati
Department of Physics, Carnegie-Mellon University, Pittsburgh, Pennsylvania 15213
and The James Franck Institute, The University of Chicago, Chicago, Illinois 60637

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The $O(n)$ model consisting of n-component spins $\vec{S}$ with the constraint $\vec{S}^2=\lambda$ in a magnetic field h is studied. It is shown that mathematically it is possible for the susceptibility to become negative for $n<1$, which implies a violation of convexity properties for $n<1$. In a mean-field approximation, the susceptibility χ_n and the specific heat C_n are positive near the critical temperature T_c for all $n \geq 0$ in contradiction with the ϵ expansion, but they become negative at very low temperatures for $n<1$. It is also shown that the spontaneous magnetization is not a monotone function of temperature for $n<1$. Our calculation also supports the conclusion drawn by des Cloizeaux that the low-temperature phase of the $O(0)$ model describes the semidilute regime of the polymer system as $h \to 0$.

The $O(n)$ model consisting of classical n-component spins $\vec{S}=\{S^{(\alpha)}, \alpha=1, \ldots, n\}$ has played a very important role in the modern statistical mechanics of phase transitions and critical phenomena. While this model is defined in a natural way for all positive integers n, it is of interest to also consider what happens for other values of n. In particular, as has been pointed out by de Gennes[1] and des Cloizeaux,[2] the limit as $n \to 0$ corresponds to self-avoiding walks,[3–5] and is hence of interest as a model of polymers.

However, this model seems to exhibit certain thermodynamic peculiarities for $n<1$. Balian and Toulouse[6] have shown that the heat capacity C_n for a one-dimensional chain becomes negative at very low temperatures for $n<1$. For the same values of n, the longitudinal susceptibility χ_n calculated in an ϵ expansion ($\epsilon=4-d$) (Refs. 7 and 8) becomes negative at temperatures T below the critical temperature T_c in the limit as the magnetic field vanishes.[9] Negative values of these quantities violate the standard convexity conditions of equilibrium statistical mechanics, conditions[10,11] which are surely fulfilled for any integer $n \geq 1$. In addition, Wheeler and Pfeuty[12] have argued that at $n=0$ the convexity conditions must be violated above T_c if scaling is obeyed. On the other hand, Moore and Wilson[9] have argued on physical grounds that χ_n must be positive and have produced an approximate calculation in which this is indeed the case.

In this paper, we shall study the thermodynamic properties of the $O(n)$ model by studying a single site in a magnetic field, a mean-field approximation to the many-site problem, and by examining the ground-state energy as a function of n. The first of these exhibits a negative χ_n (in large field h) for any $n<1$, contrary to Moore and Wilson.[9] The mean-field calculation produces a positive χ_n and C_n near $T=T_c$ for all n as $n \to 0$, in contrast to the ϵ expression, but both quantities become negative at sufficiently low temperatures for $n<1$ ($h \to 0$). In addition, the spontaneous magnetization m_n is not a monotone decreasing function of T for $n<1$, and for $\vec{s}^{\,2} n=0$, m_n is actually zero at $T=0$. That this last result, which has not previously been pointed out, is not simply an artifact of the mean-field approximation is supported by a consideration of the ground-state energy. While convexity does not imply that m_n must decrease with T, the inequalities of Griffiths[13] and Ginibre[14] imply that this is the case for $n=1$ and 2, and it is believed to be true for integer $n \geq 3$. The presence of these anomalies suggests that the $O(n)$ model for $n<1$ may be quite different from $n \geq 1$. However, we have other arguments (to be presented elsewhere) which suggest that certain violations of convexity can also occur for $n>1$ when n is not an integer.

Consider a single spin $\vec{S}=\{S^{(\alpha)}, \alpha=1, \ldots, n\}$ in a magnetic field h along the $\alpha=1$ direction. Throughout this paper, we will assume that the length of the spin is constrained: $\vec{S}^2=\lambda$. Then the partition function involves only the angular integration over $d\Omega_n$ and is given by ($H = h/T$, and the Boltzmann constant $k_B = 1$)

$$z_n = \int d\Omega_n e^{HS^{(1)}} \Big/ \int d\Omega_n$$
$$= \Gamma(n/2) \left[\frac{\sqrt{\lambda} H}{2} \right]^{1-(n/2)} I_{(n/2)-1}(\sqrt{\lambda} H) ,$$

where $I_\nu(x)$ is the modified Bessel function of order ν. The magnetization m_n is given by

$$m_n = y_n(H,\lambda) = \sqrt{\lambda} I_{n/2}(\sqrt{\lambda} H) / I_{(n/2)-1}(\sqrt{\lambda} H) , \quad (1)$$

which also defines $y_n(H,\lambda)$. For $H << 1$, $m_n = H + O(H^3)$ while for $H >> 1$, we have

$$m_n = \sqrt{\lambda} - (n-1)/2H + O(1/H^2) . \quad (2)$$

It is evident from (2) that the susceptibility $\chi_n = (n-1)/(2TH^2) + O(1/H^3)$ and becomes negative for $n < 1 (H >> 1)$, while it remains positive for $H << 1$. The behavior of m_n is shown schematically in Fig. 1 for $n \geq 1$ and $0 < n < 1$ separately: we note that m_n, i.e., y_n is not monotonic for $n < 1$.

The Hamiltonian of the system of N spins is given by

$$\mathscr{H}_n = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j - h \sum_i S_i^{(1)} ,$$

where $J > 0$ and h is the external magnetic field in the $\alpha = 1$ direction which breaks the $O(n)$ symmetry of the first term, and the length of each spin $\vec{S}_i$ is constrained: $\vec{S}_i^2 = \lambda$. We will be considering the following two cases: (a) $\lambda = n$ and (b) $\lambda = 1$. The analogy with the polymer system is obtained for $\lambda = n$.[3–5] At first it appears that the two cases are very different in the $n \to 0$ limit. However, we will see below that they both belong to the *same* universality class.

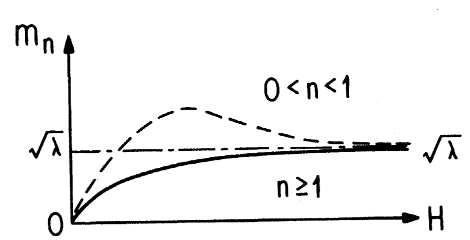

FIG. 1. The curves for m_n or y_n. The solid curve is for $n \geq 1$ and the broken curve is for $0 < n < 1$.

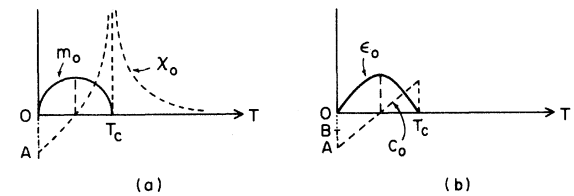

FIG. 2. The case $\lambda = n$. χ_0 and C_0 are *negative* below $T = T_c/2$.

The ground-state energy $E_g(\lambda)$ of $\mathscr{H}_n$ is given by

$$E_g(\lambda) = -N(Jq\lambda/2 + \sqrt{\lambda} h) , \quad (3)$$

where q is the coordination number of the lattice. This is the energy of the system at $T = 0$. Let $e_n(T,\lambda)$, $m_n(T,\lambda)$, and $\chi_n(T,\lambda)$ denote the internal energy, the magnetization, and the susceptibility per particle, respectively. Setting $h = 0$ we obtain from Eq. (3)

$$T = 0: \; e_n = -Jq\lambda/2, m_n = \sqrt{\lambda}, \chi_n = 0 \quad (4)$$

(see Figs. 2 and 3 for details for $n \to 0$). It should be remarked that the derivation of (4) is *not* based on any approximations.

For $\lambda = n$, $m_0 = 0$ for $n = 0$ at $T = 0$. Therefore, it is possible that (i) $m_0(T,0)$ remains zero everywhere with some singularity at $T = T_c$ and is indeed the case in one dimension,[5] or (ii) $m_0(T,0)$ has a "humplike" behavior between $T = 0$ and $T = T_c$ as shown in Fig. 2(a). We will now show that at least in the mean-field approximation, $m_n(T,\lambda)$ is not a monotone decreasing function of T. For this, we rewrite $\mathscr{H}_n$ in the following way:

$$\mathscr{H}_n = -\sum_{\langle ij \rangle} \vec{S}_i' \cdot \vec{S}_j' - \sum_i \vec{S}_i \cdot (Jq\vec{m}_n + \vec{h}) + \tfrac{1}{2} NJq\vec{m}_n^2$$

where $\vec{m}_n = \vec{m}_n(T,\lambda)$ is the average magnetization

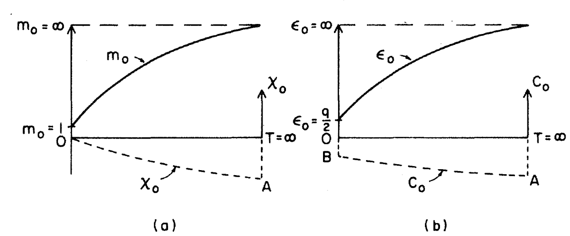

FIG. 3. The case $\lambda = 1$. m_0 and ϵ_0 are monotonically increasing functions and become infinite as $T \to T_c = \infty$; χ_0 and C_0 are *always negative.*

per particle and $\vec{S}_1'=\vec{S}_i-\vec{m}_n$. In the mean-field approximation, we neglect the first term. Then the free energy per particle $\omega_n(T,\lambda)$ equal to $\ln Z_n/N$ in the limit $N\to\infty$, where Z_n is the partition function, is given by

$$\omega_n(T,\lambda)=-\frac{(\vec{\sigma}-\vec{H})^2}{2Kq}+\ln\Gamma(n/2)(\sqrt{\lambda}\sigma/2)^{1-n/2}I_{n/2-1}(\sqrt{\lambda}\sigma)\ ,$$

where $\vec{\sigma}=Kq\vec{m}_n+\vec{H}$, $K=J/T$, and $\vec{H}=\vec{h}/T$. Minimizing ω_n with respect to σ, we find that m_n is given by

$$m_n(T,\lambda)=(\sigma-H)/Kq=y_n(\sigma,\lambda)\ . \tag{5}$$

For $h=0$, one is looking for the intersection of $y=\sigma/Kq$ and $y=y_n(\sigma,\lambda)$. It is evident from Fig. 1 that (i) $m_n(T=0,\lambda)=\sqrt{\lambda}$, and (ii) $m_n(T,\lambda)$ is *not* a monotone decreasing function of T for $n<1$. In the following, we will be chiefly interested in the case $n\to 0$. Moreover, we will be considering the limit $h\to 0$.

Setting $\lambda=n$ and taking $h\to 0$ limit in Eq. (5), we find that the spontaneous magnetization $m_0=m_0(T,0)$ for $n\to 0$ is given by

$$m_0=Kqm_0/[1+(Kqm_0)^2/2] \tag{6}$$

and has the following nonzero solution ($T_0=T_c=Jq$):

$$m_0(T,0)=(1/T_0)\sqrt{2T(T_c-T)},\ T<T_c\ .$$

For $T>T_c$, $m_0(T,0)=0$ [see Fig. 2(a)]. The susceptibility is given by

$$\chi_0(T,0)=\begin{cases}1/(T-T_c), & T>T_c\\ (1/2T_0)(2T-T_c)/(T_c-T), & T<T_c\end{cases}$$

[see the dashed curve in Fig. 2(a)]. The *most important observation* is that $\chi_0(T,0)<0$ for $T<T_c/2$. For $T>T_c/2$, $\chi_0(T,0)>0$. For $T\to 0+$, we find that $\chi_0(T\to 0+,0)=-1/2T_0$. However, for $T=0$, we know from Eq. (4) that $\chi_0(T=0,0)=0$ and this explains the portion OA in Fig. 2(a). The energy per particle $\epsilon_0(T,0)=\partial\omega_0/\partial K$ (ϵ_0 is related to the usual energy per particle e_0 via $\epsilon_0=-e_0/J$) is given by [see the solid curve in Fig. 2(b)]

$$\epsilon_0(T,0)=(T/J)(1-T/T_c)\geq 0\quad (T<T_c)\ .$$

At $T=0$, ϵ_0 agrees with the result $e_0(T=0,0)=0$. The specific heat $C_0(T,0)$ is

$$C_0(T,0)=(1-2T/T_c),\quad T<T_c$$

and shows clearly that $C_0(T,0)<0$ for $T<T_c/2$. The behavior of $C_0(T,0)$ is shown schematically by the dashed curve in Fig. 2(b). It is easily seen that for $T>T_c$, $\epsilon_0=0$, and $C_0=0$. As $T\to 0+$, $C_0(T,0)\to -1$. However, it can be shown that for any arbitrary n, $C_n(T=0,0)=-(1-n)/2$. Thus, $C_0(T=0,0)=-1/2$ and this explains the portion AB of the curve in Fig. 2(b). It is easily seen that χ_n and C_n remain negative near $T=0$ for $0<n<1$. However, as $n\to 1$, these negative portions disappear and χ_n and C_n become positive for all T. Near $T=T_c$, they remain positive for all n.

Setting $\lambda=1$ and taking the $h\to 0$ limit in Eq. (5), we find that $m_0(T,1)$ must satisfy

$$m_0=I_0(Kqm_0)/I_{-1}(Kqm_0)\ . \tag{7}$$

Equation (7) always has a nonzero solution for all values of T, i.e., there is a phase transition at infinite temperature $T_0=\infty$. The curve for $m_0(T,1)$ starts at unity at $T=0$ and rises steadily until it approaches infinity as $T\to T_c=\infty$ [see the solid curve, Fig. 3(a)]. The susceptibility near $T=0$ is $\chi_0(T,1)=-T/[2T_0(2T_0+T)]$ whereas as $T\to\infty$, $\chi_0(T,1)=-1/2T_0$, and is shown schematically by the dashed curve in Fig. 3(a).

The behavior of this model with $\lambda=1$ can easily be understood in terms of the model with $\lambda=n$ by observing that the two systems are *identical* under the following mappings: $\vec{S}(1)=\vec{S}(n)/\sqrt{n}$, $K(1)=nK(n)$, and $H(1)=\sqrt{n}H(n)$, where the arguments n or 1 refer to the two cases (a) $\lambda=n$ or (b) $\lambda=1$. Thus, the two cases belong to the *same* universality class. We note that $m_n(T(1),1)=m_n(T(n),n)/\sqrt{n}$ which ensures that $m_n(T=0,1)=1$ [see Eq. (4)]. We also observe that the temperature scales of the two systems are related via $T(1)=T(n)/n$. The critical temperatures of the two systems are therefore related through $T_c(1)=T_c(n)/n$. It should be evident that a vanishingly small neighborhood around $T(n)=0$ is mapped onto the whole $T(1)$ axis [except a vanishingly small neighborhood around $T(1)=\infty$] and the rest of the $T(n)$ axis is mapped onto the above vanishingly small neighborhood around $T(1)=\infty$ as $n\to 0$. It is easily shown that $\chi_n(T(1),1)=\chi_n(T(n),n)$. This implies that the portion OA in Fig. 2(a) has been mapped onto the portion OA in Fig. 3(a) covering the "whole" temperature range [except a vanishingly small neighborhood around $T(1)=\infty$]:

$$\chi_0(T\to 0+,0)=\chi_0(T\to\infty,1)=-1/2T_0\ .$$

The rest of the curve in Fig. 2(a) has been mapped on at infinity in Fig. 3(a).

One can also show that $C_n(T(1),1)=C_n(T(n),n)$. Thus, the specific heat also becomes negative for $n=0$, similar to case (a). The functions $\epsilon_0(T,1)$ and $C_0(T,1)$ are shown by the solid and the dashed curves in Fig. 3(b). At $T=0$, $\epsilon_0(T=0,1)=q/2$ and agrees with the result that $e_0(T=0,1)=-Jq/2$ [see (4)] (remember that $\epsilon_0=-e_0/J$) and $C_0(T=0,1)=-1/2$. As $T\rightarrow T_c=\infty$, $\epsilon\rightarrow\infty$ and $C_0\rightarrow -1$. Thus, the portion AB of Fig. 2(b) has been mapped onto the "whole" portion AB in Fig. 3(b).

Before we end, we wish to consider the relevance of our mean-field calculation for the polymer system.[3-5] As $h\rightarrow 0$ the polymer density $\phi_l=K\epsilon_0(T,0)=1-T/T_c$ and the polymer chain density $\phi_p\rightarrow 0$ for $T\leq T_c$. Therefore, in the mean-field approximation used here, we find that the semidilute regime characterized by $\phi_l<<1$ and $\phi_p\rightarrow 0$ is described by a small-temperature regime defined by $T=T_c(1-\phi_l)$ as $h\rightarrow 0$. In this respect, our analysis seems to provide a support for the conclusion drawn by des Cloizeaux[2] that the low-temperature phase of the $O(0)$ model provides a description of the semidilute regime in the limit $h\rightarrow 0$. This is very important since the analogy between the polymer system and the $O(0)$ model has been established only at high temperatures where the series expansion makes sense.[3-5]

Let us briefly summarize our important results for $n<1$. We have shown that the spontaneous magnetization is not a monotone function of T. For $\lambda=n=0$, m_n is identically zero at $T=0$. This observation is independent of the mean-field approximation. If one believes that m_n is nonzero just below T_c and is a continuous function of T, then there must be a range of T near $T=0$, where m_n is increasing with T for $n=0$. Thus, m_n is not a monotone function of T for $n=0$. The mean-field calculation shows this to be the case for all $n<1$. It will be reported elsewhere that the spin-wave analysis predicts that m_n is an increasing function of I for $n<1$ and a decreasing function of I for $n>1$ near $T=0$. This confirms the mean-field result given above. Also χ_n and C_n can indeed become negative. However, near $T=T_c$, they both are positive, in contrast to the ϵ expansion. It is conceivable that the mean-field approximation is not physically meaningful. But then again, it is conceivable that the ϵ expansion can not be trusted for $n<1$. The arguments of Wheeler and Pfeuty[12] are valid if the critical exponent $\gamma>1$. In the mean field, $\gamma=1$; therefore, their proof does not work. However, if the real system does have positive χ_0 and C_0 near T_c as the mean field implies, one might have to abandon scaling for $n=0$.

Note added in proof. Recently, Wheeler and Pfeuty[15] have also independently noted the nonmonotonicity of m_n for $n\rightarrow 0$.

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