Critical Behavior of the n-Vector Model with a Free Surface

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Correlation-function exponents $\eta_\perp$ and $\eta_\parallel$ appropriate to the free-surface problem have been obtained by renormalization-group calculation to order ϵ^2. By using the scaling relations $\gamma_1 = \nu(2-\eta_\perp)$ and $\gamma_{11} = \nu(1-\eta_\parallel)$, expansions for γ_1 and γ_{11} are obtained. These expansions are in agreement with the surface scaling relation $2\gamma_1 - \gamma_{11} = \gamma + \nu$, but disagree with the relation $\gamma_{11} = \nu - 1$ due to Bray and Moore.

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A number of authors[1-11] have recently studied the critical behavior of the semi-infinite n-vector model. New critical exponents appropriate to the surface problem have been variously defined,[3,6] and scaling relations between these exponents have been obtained.[3,6] The correlation-function exponents $\eta_\perp$ and $\eta_\parallel$ were introduced by Binder and Hohenberg,[3] as were the layer and local susceptibility exponents γ_1 and γ_{11}. The exponents $\eta_\perp$ and $\eta_\parallel$ are defined via the real-space spin-spin correlation function $G(\rho, z, z')$, where ρ is a $(d-1)$-dimensional vector giving position vector coordinates in a plane parallel to the surface, while z and z' are coordinates perpendicular to the surface. The definitions are $G(\rho,z,z') \sim \rho^{2-d-\eta_\parallel}$ as $\rho \to \infty$, with z and z' fixed, and $G(\rho,z,z') \sim (z')^{2-d-\eta_\perp}$ as $z' \to \infty$, with ρ and z fixed. An additional magnetic field term H', which couples only to surface spins, permits the identification of layer and local susceptibilities, $\chi_1 \sim -\partial^2 A/\partial H\,\partial H'$ and $\chi_{11} \sim -\partial^2 A/\partial H'^2$, respectively, where A is the Gibbs free energy and H is the bulk field. The zero-field limit of these susceptibilities permits the identification of corresponding exponents viz. $\chi_1 \sim t^{-\gamma_1}$ and $\chi_{11} \sim t^{-\gamma_{11}}$.

Lubensky and Rubin[4] calculated the exponents $\eta_\perp$ and $\eta_\parallel$ to first order in ϵ, and, through the scaling relations $\gamma_1 = \nu(2-\eta_\perp)$ and $\gamma_{11} = \nu(1-\eta_\parallel)$, also obtained the corresponding expansion for γ_1 and γ_{11}. These were subsequently verified by Reeve and Guttmann,[7] who calculated γ_1 and γ_{11} directly to first order in ϵ. Barber[6] derived the scaling relation $2\gamma_1 - \gamma_{11} = \gamma + \nu$ [hereinafter referred to as the surface scaling relation (SSR)], and in 1977 Bray and Moore[5] used an argument based on statements correct to all orders in perturbation theory to suggest the relation $\gamma_{11} = \nu - 1$ [hereinafter called the Bray-Moore surface relation (BMSR)], which implies $\eta_\parallel = 1/\nu$.

Related position-space renormalization-group calculations have been made by several authors,[8] though those calculations are not of direct relevance to the problem at hand.

As pointed out by Bray and Moore,[5] the BMSR is satisfied by the exponent values of the two-dimensional Ising model, the n-vector model to order ϵ, and the $n=\infty$ limit of the n-vector model for arbitrary dimensionality. However, series-analysis studies have cast doubt on the validity of the BMSR for some systems. Barber *et al.*[9] found that for the $n=0$, $d=2$ model $\gamma_{11} = -0.19^{+0.03}_{-0.02}$, while $\nu - 1 = 0.25$. For the $n=0$, $d=3$ model they found $\gamma_{11} = -0.35 \pm 0.05$ which is just consistent with the series value of $\nu - 1 = -0.4$. The validity of the technique which produced the observed discrepancy in the $d=2$ case was confirmed by Enting and Guttmann.[10] For the $d=3$, $n=1$ (Ising) model, Whittington, Torrie, and Guttmann,[11] assuming the SSR, obtained $\gamma_{11} = -0.33 \pm 0.04$, which is in agreement with the BMSR prediction of $\gamma_{11} = -0.362^{+0.001}_{-0.002}$. For both bond and site percolation problems on the fcc lattice De'Bell and Essam[12] obtained estimates of γ_{11} and ν which violated the BMSR. For two-dimensional percolation at a surface, the surface transition does not exist, since $\nu > 1$. De'Bell and Essam also studied the $n=0$, $d=2$ model on a different lattice to that chosen by Barber *et al.*,[9] and confirm the breakdown of the BMSR observed by Barber *et al.*

Without exception, the above-mentioned series analysis studies confirm the SSR of Barber.[6]

Given the apparent breakdown of the RGSR in several systems, as suggested by the above series studies, it was decided to extend the ϵ expansions of $\eta_\perp$ and $\eta_\parallel$ to second order in ϵ in order to determine whether the BMSR still held.

Following the formulation of Lubensky and Rubin,[4] the Hamiltonian (in the momentum representation) for a semi-infinite $O(n)$ system in d dimensions can be written

$$H = \tfrac{1}{2}\int d\bar{q}(m^2+q^2)\varphi_i(\bar{q})\varphi_i(\nu\bar{q}) + \tfrac{1}{8}(g_0/4!)\sum_{\{\epsilon_i=\pm1\}}\epsilon_1\epsilon_2\epsilon_3\epsilon_4\int\Big(\prod_i d\bar{q}_i\Big)\varphi_i(\bar{q}_1)\varphi_i(\bar{q}_2)\varphi_j(\bar{q}_3)\varphi_j(\bar{q}_4)\,\delta\Big(\sum_i p_i\Big)\,\delta\Big(\sum_i \epsilon_i k_i\Big), \quad (1)$$

where $\bar{q}=(\bar{p},k)$, $\bar{p}$ being a $(d-1)$-dimensional vector, $\nu\bar{q}=(-\bar{p},k)$, and the Fourier expansion functions are

$$\psi_q(x)=\sqrt{2}\exp(i\vec{p}\cdot\vec{\rho})\sin(kz), \qquad (2)$$

by assuming that the spin interaction strength in the surface is the same as in the bulk.[13] The real-space variables are $x=(\bar{\rho},z)$, where $\bar{\rho}$ is a $(d-1)$-dimensional vector and the surface boundary is located at $z=1$. The propagator for the system at the bulk critical point, $m^2=0$, is $G_p^{(0)}(k_1,k_2) = [\delta(\bar{q}_1-\nu\bar{q}_2)-\delta(\bar{q}_1+\bar{q}_2)]/2q_1^2$, where $\bar{q}_1=(\bar{p},k_1)$ and $\bar{q}_2=(\bar{p},k_2)$.

We have extended[4] the $\epsilon=4-d$ expansion for the two-point Green's function $G_p(k_1,k_2)$ to second order by expanding to two loops and calculating diagrams within the framework of dimensional regularization.[14] The finite quantity $G_p^R(k_1,k_2)$ is found by minimal subtraction[14] of poles in ϵ from $G_p(k_1,k_2)$. The two quantities are related by $G_p(k_1,k_2)=ZG_p^R(k_1,k_2)$. Since all the poles in ϵ contained in the wave-function renormalization, Z, originate only from the momentum conserving or "bulk" terms in $G_p(\boldsymbol{k}_1,k_2)$, the diagonal part of $G_p(k_1,k_2)$ which is $G_p(k_1,k_2)[\delta(\bar{q}_1-\nu\bar{q}_2)-\delta(\bar{q}_1+\bar{q}_2)]/2q_1^2$ obeys the usual renormalization-group equation.[14] Consequently, and because the mass and coupling-constant renormalization functions remain exactly as for the bulk system, the bulk exponents can be calculated in the usual way. The renormalized coupling constant and its fixed-point value can be taken from the calculation for the infinite system, and we have gleaned these quantities directly from Amit[14] after suitably matching conventions. The $G_p^R(k_1,k_2)$ are inverse Fourier transformed to give $G_p(z_1,z_2)$ in the mixed space.

The decay of the correlations of spins in the boundary surface is assumed to be $G_p^R(1,1) \sim p^{-1+\eta_\parallel}$ and the asymptotic form of the bulk-spin–surface-spin correlations is assumed to be $G_p^R(1, z_2\to\infty)\sim p^{-2+\eta_\perp}$, as $p\to 0$. [In fact, we have calculated $\sum_{z_2\geq 1} G_p^R(1,z_2)$, which is reasonable to assume has the same asymptotic form as $G_p^R(1,z_2\to\infty)$.] The critical exponents $\eta_\parallel$ and $\eta_\perp$ are identified by exponentiation. The results are

$$\eta_\parallel = 2-\frac{n+2}{n+8}\epsilon-\frac{(n+2)(17n+76)}{2(n+8)^3}\epsilon^2 \qquad (3)$$

and

$$\eta_\perp = 1-\frac{n+2}{2(n+8)}\epsilon-\frac{(n+2)(4n+17)}{(n+8)^3}\epsilon^2. \qquad (4)$$

From the scaling relations $\gamma_1=\nu(2-\eta_\perp)$ and $\gamma_{11}=\nu(1-\eta_\parallel)$, and the known expansion for ν, given by

$$\nu=\tfrac{1}{2}+\frac{n+2}{4(n+8)}\epsilon+\frac{(n+2)(n^2+23n+60)}{8(n+8)^3}\epsilon^2, \qquad (5)$$

we obtain

$$\gamma_1=\tfrac{1}{2}+\frac{n+2}{2(n+8)}\epsilon+\frac{(n+2)(2n^2+49n+144)}{8(n+8)^3}\epsilon^2 \qquad (6)$$

and

$$\gamma_{11}=-\tfrac{1}{2}+\frac{n+2}{4(n+8)}\epsilon+\frac{(n+2)(n^2+31n+124)}{8(n+8)^3}\epsilon^2. \qquad (7)$$

By inspection one sees that the BMSR of Bray and Moore[5] is violated at order ϵ^2; i.e., $\gamma_{11}\neq\nu-1$, while using the known expansion for γ, given by

$$\gamma=1+\frac{n+2}{2(n+8)}\epsilon+\frac{(n+2)(n^2+22n+52)}{4(n+8)^3}\epsilon^2, \qquad (8)$$

one finds that the SSR of Barber,[6] $2\gamma_1-\gamma_{11}=\gamma+\nu$, is satisfied. This last result provides a particularly valuable consistency check on our results. The Fourier transforms required in evaluating

TABLE I. Sums to order ϵ and ϵ^2 of γ_1 and γ_{11} compared with the best series estimates. Values marked with an asterisk are exact.

		γ_1			γ_{11}		
n	Dimensionality d	Sum to order ϵ	Sum to order ϵ^2	Best series estimate	Sum to order ϵ	Sum to order ϵ^2	Best series estimate
0	2	0.75	1.031	0.945[a]	−0.375	−0.133	−0.19[a]
1	2	0.833	1.235	1.375*	−0.333	−0.012	0.00*
0	3	0.625	0.695	0.70[a]	−0.438	−0.377	−0.35[a]
1	3	0.667	0.767	0.78[b]	−0.417	−0.336	−0.33[b]

[a]Ref. 8.
[b]Ref. 10.

$\eta_{\parallel}$ and $\eta_{\perp}$ are quite independent, and hence so are the expansions for $\eta_{\perp}$ and $\eta_{\parallel}$. That these independent expressions give rise to expansions that satisfy the SSR is greatly reassuring.

In order to see the effect of these new terms in the ϵ expansion for γ_1 and γ_{11}, we show in the accompanying Table the sums to order ϵ and order ϵ^2 of γ_1 and γ_{11} as well as the best series estimates. In every case the $O(\epsilon^2)$ term has effected a substantial improvement over the sum to $O(\epsilon)$, and in three dimensions all sums to $O(\epsilon^2)$ are within 3% of the series estimates. The agreement obtained by using $\gamma_{11} = \nu - 1$ and summing to $O(\epsilon^2)$ is significantly worse.

We conclude that surface scaling is well supported by our calculations, but that the relation $\gamma_{11} = \nu - 1$ due to Bray and Moore is incorrect.

After submission of this Letter, we became aware of the recent calculations of Diehl and Dietrich,[15] who confirm our result for $\eta_{\parallel}$ by an alternative calculation. They have also derived the scaling laws for surface exponents.

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Infinite Susceptibility Phase in Random Uniaxial Anisotropy Magnets

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The leading terms in the magnetic equation of state are calculated for models with random fields and random uniaxial anisotropies for dimensionalities $d<4$. In the random anisotropy case we find a new low-temperature phase, in which the magnetization vanishes but the zero-field susceptibility is infinite, because of algebraically decaying correlations. No phase transition is found for the random field case.

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It has recently been realized theoretically that when fluctuations are taken into account, then various types of randomness destroy long-range magnetic order in Heisenberg-like systems ($m > 1$ spin components) with realistic dimensionalities $d<4$. Of particular interest are systems with (a) *random magnetic fields*,[1] where the randomness enters via

$$\sum_x [\vec{h}(x)\cdot\vec{S}(x)],\quad [\vec{h}(x)]_{av}=0,\quad [|\vec{h}(x)|^2]_{av}=\Delta,$$

and (b) *random uniaxial anisotropy*,[2] where the randomness arises via $-D\sum_x[\hat{n}(x)\cdot\vec{S}(x)]^2$, where $\hat{n}(x)$ is a unit vector with random direction. Sys-