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Universality of surface critical behavior of the three-dimensional Ising model in a random surface field

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The Harris criterion is generalized to determine the relevance at bulk criticality (in the scaling theory sense) of a random ordering field acting at a surface only. For surface critical behavior of the three-dimensional Ising model the criterion predicts the random field to be irrelevant for the ordinary transition, and relevant for the surface-bulk multicritical point. Monte Carlo results for the ordinary transition verify the prediction. Moreover, surface critical behavior near substrates chemically altered in part, as used in a series of experiments by Franck and co-workers, is in the universality class mentioned above, and the value of β_1 found in a random surface experiment [D. J. Durian and C. Franck, Phys. Rev. Lett. **59**, 555 (1987)] agrees with the scaling prediction.

INTRODUCTION

Magnetic systems in the presence of a random field have been studied rather extensively in recent years, both theoretically and experimentally. In this paper we address a related problem, namely, a three-dimensional Ising model with a random field acting only at its surface. In studying this problem we are motivated by a series of recent experiments on wetting and critical adsorption of binary mixtures on chemically tunable substrates.[1,2]

In the experiment directly relevant for our discussion, Durian and Franck consider a binary mixture of a polar liquid (nitromethane) and a nonpolar liquid (carbon disulfide) in the two-phase region below the critical mixing temperature.[2] They measured the wetting temperature of this mixture, using a series of substrates (borosilicate glass) with polarities varied chemically (decreasing with degree of silylation). The phase relatively richer in the polar component completely wets the clean substrate. By decreasing the polarity of the surface, and thereby decreasing the preference of the wall for the wetting phase, the wetting temperature is driven up continuously to the bulk critical-mixing temperature. Close to this temperature, measurement of the contact angle as a function of temperature allowed Durian and Franck to obtain an estimate of the critical exponent β_1-μ, where β_1 and μ are the exponents of the surface-order parameter (m_1) and surface tension, respectively. Actually, the exponent β_1 in this experiment describes the surface-order parameter in the presence of a random-ordering field of vanishing average strength acting at the surface only. The experimental estimate of the exponent agrees with experimental[3] and theoretical values[4,5] for systems in the Ising universality class without a surface-ordering field, indicating that the random surface field is irrelevant in the scaling theory sense. In this paper we address the question of relevance of the random surface field for the three-dimensional Ising model. First, a simple argument shows that indeed surface randomness is irrelevant for the case of the ordinary transition in the three-dimensional Ising model. Second, Monte Carlo results are presented which support this prediction.

MODEL AND METHOD

The critical behavior of the binary mixture mentioned above is in the universality class of the three-dimensional Ising model. Partial chemical alteration of the substrate is modeled by a quenched random surface field. We consider a finite system of $n\times n\times m$ sites $i=(x,y,z)$, where x, y, and z are integers with $1\leqq x\leqq n$, $1\leqq y\leqq n$, and $1\leqq z\leqq m$. There are two surfaces, one at $z=1$ and the other at $z=m$. All sites that are not on the surface will be referred to as bulk sites. The system is chosen to have periodic boundary conditions in the x and y directions.

The Hamiltonian H in units kT is given by

$$-\frac{H}{kT}=K\sum_{(i,j)}s_is_j+K_s\sum_{(i,j)}s_is_j+\sum_i h_is_i \ . \qquad (1)$$

Here, the first and second summations are over all nearest-neighbor pairs of sites (i,j) such that in the first sum at least one of the sites is in the bulk and in the second sum both are on a surface. The third sum is over single sites at the surface. In Eq. (1) K and K_s are the nearest-neighbor bulk and surface coupling constants. The random field h_i assumes values $+h_r$ and $-h_r$ uncorrelated from site to site; the field sums to zero on each surface. All our calculations were performed at $K=0.2217$,[6] the bulk critical coupling, and $K_s=K/2$. The strength of the random field, h_r, was varied between zero and twice the bulk coupling K.

The spin-spin correlation function $g(r)$ for two spins on the same surface at distance r is defined as

$$g(r)=\langle\langle s_is_j\rangle-\langle s_i\rangle\langle s_j\rangle\rangle_r \ , \qquad (2)$$

where $\langle\cdots\rangle$ indicates a thermal average, and $\langle\cdots\rangle_r$

stands for the average over the random surface field. According to finite-size scaling, at bulk criticality the correlation function satisfies the following scaling relation:

$$g(r) \sim b^{-2x_r} g(r/b) \ , \qquad (3)$$

where b is an arbitrary length rescaling factor, and x_r is the critical dimension of surface magnetization. The exponent x_r is related to β_1, the exponent describing the spontaneous surface magnetization via $\beta_1 = x_r \nu$. Note that under rescaling, a nonzero average surface field h_r rescales to $b^{y_r} h_r$, where $x_r + y_r = d'$ for a surface dimensionality d'. In particular, it follows from Eq. (3) that

$$g(n/2) \sim n^{-2x_r} \ . \qquad (4)$$

This relation was used (following Ref. 7) in the estimation of the surface magnetic critical exponent x_r from the Monte Carlo data for the surface correlations at criticality as a function of system size n. In our calculations, pairs of surface spins separated by a displacement $n/2$ along the x axis, the y axis, or diagonally, were included with equal weights in $g(n/2)$.

IRRELEVANCE OF THE RANDOM FIELD

When is the exponent x_r in Eq. (3) the same as the corresponding exponent x_{H_1} for the Ising model with a free surface? Following Andelman and Berker[8,9] we derive how a random field of strength h_r rescales under a renormalization transformation with a spatial change of scale b. First, the field, varying randomly over the spins in a Kadanoff block at the surface, is replaced by a field of strength $b^{d'/2}$ uniform on the surface of the block. Then, relying on the local nature of the renormalization transformation, this field rescales for single blocks as a *uniform* surface field with scaling index y_{H_1}, i.e., by a factor $b^{y_{H_1}}$. For small random fields the net effect of these two changes is multiplicative, so that we expect the strength h_r of the random field to rescale to $b^{y_{H_1} - d'/2} h_r$. As a consequence, the random field is relevant (i.e., grows under renormalization) if $y_{H_1} \geqq d'/2$, and *vv*. For the ordinary transition of the Ising model[4,5] one has $y_{H_1} \approx 0.75$, so that the random surface field is expected to be irrelevant in this case, as implied by Durian and Franck's experiment[2] and corroborated by our Monte Carlo calculations. We also note that for the special surface transition (i.e., the surface-bulk multicritical point), for which $y_{H_1} \approx 1.72 > d'/2$,[4] the random field is expected to be relevant. A formulation analogous to the original Harris criterion is to restate the above result as follows: If γ_{11}, the exponent governing the behavior of the susceptibility of the surface layer associated with a surface field, is positive, then the random field is relevant, and *vv*. This follows immediately, since $\gamma_{11} = (2y_{H_1} - d')\nu$.

MONTE CARLO RESULTS

To check the irrelevance of the random surface field we performed a standard Monte Carlo calculation. Typically, 100 000 flips per spin were done for systems of n by n by $2n$ lattice sites. Following Binder and Landau,[4] in some of the calculations the surface spins were sampled preferentially, at a rate of ten times the bulk spins. The average over the random field involved of the order of ten independent realizations. We extracted critical exponents from the correlation function data (see Table I) by doing least-squares fits of log g vs log n. A separate fit was made for the zero-field case; the data for systems with different, nonzero random field were fitted with a single exponent. Depending on system sizes considered, the results and estimated standard errors are (1) $y_{H_1} = 0.705 \pm 0.026$ and $y_r = 0.585 \pm 0.040$ in the range $4 \leqq n \leqq 16$; (2) $y_{H_1} = 0.787 \pm 0.026$ and $y_r = 0.773 \pm 0.045$ in the range $6 \leqq n \leqq 16$; and (3) $y_{H_1} = 0.787 \pm 0.048$ and $y_r = 0.763 \pm 0.074$ in the range $8 \leqq n \leqq 16$. First, these results seem to indi-

TABLE I. Surface correlations $g(h_r)$ as a function of random field strength (expressed in units of the surface coupling K_s) for various system sizes n. The estimated standard errors in the last digits are given in parentheses.

n	$g(0)$	$g(2)$	$g(4)$
4	0.0429(16)	0.0265(12)	0.0076(14)
6	0.01384(74)	0.0070(12)	0.0017(4)
8	0.00693(39)	0.0035(5)	0.00092(32)
10	0.0038(8)	0.0016(5)	0.00053(15)
12	0.0027(3)	0.0012(4)	...
16	0.00117(22)	0.00063(13)	0.00018(13)

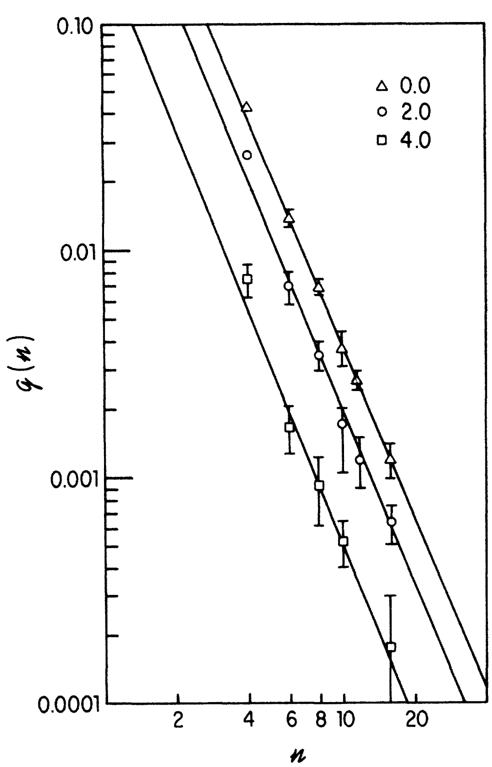

FIG. 1. Log-log plot of the two-spin correlation function at half system size with standard errors.

cate, as illustrated by Fig. 1, that within the statistical error all our system sizes except $n=4$ are in the asymptotic finite-size-scaling regime. Second, within our resolution the random field is indeed irrelevant as predicted. Finally, using all our data to estimate $y_{H_1}=y_r$, we find $y_{H_1}=0.78\pm0.02$, in the range $6\leqq n\leqq 16$ in agreement with a previous Monte Carlo result $y_{H_1}=0.76\pm0.03$,[4] and the ϵ-expansion estimate 0.75 ± 0.02.[5]

Note added. The work of Ref. 10, regarding the order of the wetting transition in the presence of surface randomness, is relevant for the experiment.[2]

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