Monte Carlo study of the surface special transition in the XY model in three dimensions

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Using extensive Monte Carlo simulations we studied the behavior of $L \times L \times D$ films containing classical spins interacting via nearest-neighbor XY interaction. Applying finite-size-scaling analysis and the cumulant method to determine the position of the surface transition boundary, we locate the multicritical point and extract appropriate critical exponents. We present evidence that the surface transition is of the Kosterlitz-Thouless type.

I. INTRODUCTION

The past two decades have witnessed a growing interest in critical properties at surfaces of physical systems in the vicinity of their bulk critical point.[1,2] In the early seventies, Binder and Hohenberg published two papers[3] in which they examined the behavior of Ising and Heisenberg films with nearest-neighbor coupling which could be modified in the surface layers with respect to that in the bulk. The authors have shown that for sufficiently enhanced coupling in the surface layer there can be distinct transitions in the surface and in the bulk.

A few years ago, Binder and Landau reported[4] the first precise simulation of the three-dimensional (3D) Ising system with free surfaces. They mapped out the phase structure of the model and gave a detailed description of the special transition (for a definition of different transitions see Fig. 1) associated with the presence of the multicritical point. This model was also studied by other authors[2,5] using Monte Carlo methods, high-temperature expansions, $1/n$ expansions, and renormalization-group techniques, so that at present its properties are quite well known.

Surface critical phenomena in continuous models have been studied in less detail. Especially little is known about the properties of a three-dimensional planar rotator model[2] (called sometimes the classical XY model, the name which we will adopt in the following) representing a system of classical spins constrained to rotate in the x-y plane of spin space, defined by the Hamiltonian as

$$H = -J \sum_{\substack{\text{NN} \\ \text{bulk}}} (S_{ix}S_{jx} + S_{iy}S_{jy}) - J_s \sum_{\substack{\text{NN} \\ \text{surf}}} (S_{ix}S_{jx} + S_{iy}S_{jy}) \,, \qquad (1)$$

where $\mathbf{S}_i$ is a two component unit vector in the direction of the classical magnetic moment at the lattice site i and J; J_s denote the bulk and the surface exchange constants, respectively. In the following we adopt units in which $k_B = 1$. Landau, Pandey, and Binder[6] examined the ordinary surface behavior in this model, investigating the surface layer magnetization exponent and the scaling property of the magnetization profile far from any multicritical point. In the present continuation of their study we aimed to describe the properties of the same model at the surface and special transitions.

It was suggested a few years ago[2,6-8] that the classical XY system in three dimensions should be able to support a phase with a quasi-long-range order at the surface in the presence of a disordered bulk. The line of a surface transition would be then of the Kosterlitz-Thouless type,[9] so that the transition corresponding to the presence of the multicritical point (i.e., special) would have a different nature. The validity of this scenario was recently proved rigorously by Frohlich and Pfister[10] (for a semi-infinite system); however, a detailed description of the surface critical properties in the model was beyond the scope of their work.

Our numerical study (preliminary parts of which have been presented elsewhere[11]) intended to shed more light on the properties of XY-like films in the vicinity of the surface transition and multicritical point. The main objective was to locate the shape of the phase boundary and to confirm the predictions about its nature being of the Kosterlitz-Thouless type. We were also interested in the position of the multicritical point and possible description of the special transition.

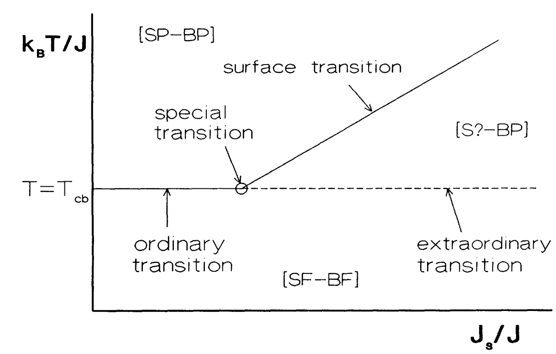

FIG. 1. Schematic phase diagram for the XY model with bulk coupling J and surface coupling J_s. The bulk transition temperature is T_{cb}. The various phases are labeled by bulk (B) and surface (S) properties as ferromagnetic (F), or paramagnetic (P). The label (S?) denotes a hypothetical Kosterlitz-Thouless surface phase (see the text).

The layout of the rest of the paper is as follows. In Sec. II we describe the method and the model, while Sec. III gives our computational results and a detailed comparison with the theoretical predictions. Section IV summarizes the main results of our study.

II. THE MODEL AND SIMULATIONAL TECHNIQUE

In our numerical study of systems described by the Hamiltonian in Eq. (1), we implemented a vectorized version of the Metropolis Monte Carlo algorithm with a checkerboard lattice decomposition[12] and layer-wise sweeps through the lattice. We used periodic boundary conditions parallel to the film; the top and the bottom were free surfaces. Since we were mainly interested in local properties of the first (and the last) layers, we decided to improve the efficiency of the program by adopting a well-known preferential sampling method:[4,6,13] Rather than sampling uniformly all the lattice, we visited the sites at the surfaces ten times more often than the sites in the bulk. For the largest systems investigated, the sampling ratio was even greater: 20:1; in the case of the small systems, it was enough to visit the surfaces seven times as often as the interior of the film.

We studied slabs with dimensions of $L\times L\times D$ with $8\le L\le 50$, and $13\le D\le 51$, respectively. We checked that this choice of D did not result in the appearance of unwelcomed finite-size effects on the properties of the surface films. Typically, after discarding about 6×10^5 Monte Carlo steps (MCS's) per layer, we performed up to 42 million MCS's/layer site for the largest systems, proportionally less for smaller ones.

All simulations were carried out on the Cyber 205 and the ETA10 supercomputers at the University of Georgia.

The important quantity which measures the intrinsic properties of the phase transition at the surface $L\times L$ is the surface layer magnetization m_1. In the vicinity of the surface transition point [with coordinates, on the phase diagram $(J_s^*/J, T_s^*/J)$], m_1 can be cast in a modified scaling form:[14,15]

$$m_1(\xi,\Delta,L)=\xi^{-\bar{\beta}}\bar{m}_1(\xi\Delta^{1/\bar{\phi}},\xi/L)\ , \tag{2}$$

where $\Delta\equiv(J_s/J_s^*-1)$, and $\bar{\phi}$ is the crossover exponent. ξ is the correlation length, which is expected to diverge in the critical regime exponentially fast:

$$\xi=a_\xi \exp(b_\xi t^{-\bar{\nu}})\ , \tag{3}$$

where a_ξ and b_ξ are constant, $t\equiv 1-T_s^*/T$, and $\bar{\nu}$ is a new exponent. Since in the limit $J_s/J\gg 1$, an effectively detached surface is equivalent to the two-dimensional (2D) XY model, one can assume that $\bar{\nu}=0.5$;[16–23] the nonuniversal parameters a_ξ and b_ξ can in principle be different than two-dimensional values.[16]

Another important quantity which we used to measure the properties of the phase transition is the fourth-order cumulant U_L,[24–29] defined as follows:

$$U_L=1-\frac{\langle m_1^4\rangle_L}{3\langle m_1^2\rangle_L^2}\ . \tag{4}$$

Here $\langle m_1^2\rangle$ and $\langle m_1^4\rangle$ denote second and fourth moments of the probability distribution of the surface magnetization $P_L(m_1)$:

$$\langle m_1^k\rangle_L=\int dm_1 m_1^k P_L(m_1)\ . \tag{5}$$

In the disordered phase, $U_L\to\frac{1}{3}$, in the ordered phase, $U_L\to\frac{2}{3}$, while at criticality, $U_L\to U^*$ (in the $L\to\infty$ limit).[6,24,25,28] For the ordinary transition, the universal constant U^* was crudely estimated to be $U^*\simeq 0.52\pm 0.04$.[6]

A convenient method for locating the transition is to record the variation of U_L with J_s/J for various L and look where these curves intersect [a similar method was chosen for a numerical study of an Ising ferromagnet with an antiferromagnetic surface layer (Ref. 8)]. Another variation of this method is to compare the values of U for two different lattice sizes, L and $L'=bL$, with the use of the condition[24–27] that

$$(U_{bL}/U_L)_{J_s=J_s^*}=1\ . \tag{6}$$

In the critical region ($\xi\gg L$), the finite-size scaling of m_1 implies that

$$m_1\simeq L^{-\bar{\beta}}\bar{m}_1(L\Delta^{1/\bar{\phi}})\ . \tag{7}$$

The surface magnetization exponent $\bar{\beta}$ can be then found by defining a function $W_{\bar{\beta}}$,[24] so that

$$W_{\bar{\beta}}=-\ln(\langle m_1^2\rangle_{bL}/\langle m_1^2\rangle_L)/\ln b\ , \tag{8}$$

and using the following formula:

$$2\bar{\beta}=(-W_{\bar{\beta}})_{J_s=J_s^*}\ . \tag{9}$$

Because of the presence of residual corrections to finite-size scaling, one actually needs to extrapolate the results of both methods as $(\ln b)^{-1}\to 0$,[24] as will be demonstrated in Sec. III.

III. RESULTS

A. Surface transition boundary

In the course of our numerical investigations, we concentrated our efforts on the precise determination of the critical coupling ratio J_s^*/J for four different values of the temperature $T/J=2.304$, 2.404, 2.500, and 3.003; we also gathered some data at $T/J=2.222$, 2.252, and 2.353. (Our preliminary runs suggested that this choice of temperatures provided phase boundary points lying reasonably close to the multicritical point.)

In Fig. 2 we show results for $U_{L'}$ plotted versus U_8 for $14\le L'\le 50$ and obtained from simulations at the temperature $T/J=3.003$. The thin solid lines show linear fits to the data close to critical surface coupling, i.e., close to the intersection with the line of slope 1. Because of corrections to scaling, the estimates for the fixed point U^* for $L=8$ depend a little bit on the scale factor $b=L'/L$, so that an additional extrapolation procedure is necessary (Fig. 3). Results of extrapolations for $L=14$, 16, 20, and 30 agree very well; the difference for $L=8$ suggests that the lattice with this small surface size is not yet in the asymptotic regime, where the effects of correction terms to finite-size scaling justify a strictly linear ex-

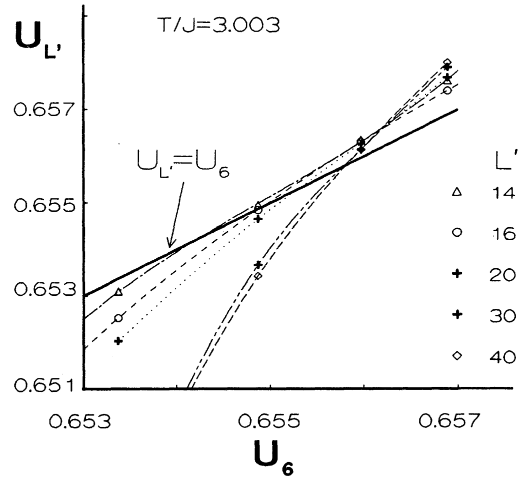

FIG. 2. The fourth-order cumulant $U_{L'}$ $(14 \le L' \le 40)$ plotted vs U_8 for $T/J=3.003$. Note the final scale of the coordinate axes, since only the data close to criticality are displayed.

trapolation.

It is crucial for the cumulants method to be successful to employ data of a very good statistical accuracy.[25] It was also evident in our simulations where enormously long Monte Carlo runs had to be used in order to obtain meaningful results (please note the scale on the cumulant axis on Fig. 2); a typical error of $U_{L'}$ was about 0.0004, i.e., two orders of magnitude smaller then the value quoted in Ref. 6.

Repeating the above procedure for each of four temperatures given above, we obtained the cumulant fixed point U^*, whose value varied slightly with T/J (Table I). We suspect that this results from the presence of additional corrections to scaling due to a finite bulk thickness. Our final estimate of U^* is $U^*_{\mathrm{KT}}=0.655\pm0.002$. For comparison we note that, for the ordinary transition,[6] $U^*=0.52\pm0.04$. On the other hand, the fixed-point value U^*, corresponding to the Kosterlitz-Thouless (KT) transition in the simple 2D XY model, is[26] $U^*_{\mathrm{KT}}=0.652\pm0.006$, in a good agreement with our present result.

As a comment on the above calculations of the fixed-point cumulant, we point out the somewhat misleading way we mentioned the crossing of surface magnetization cumulant lines corresponding to different lattice sizes. Actually, the curve U_{bL} versus U_L should (in the limit $L \rightarrow \infty$) touch the line $U_{bL}=U_L$ tangentially at J_s^*/J and move along toward the $J_s^*/J=\infty$ ("zero temperature") fixed point, $U^*_\infty \equiv \frac{2}{3}$. The fixed-point value U^* varies then between 0.655 ± 0.002 and $\frac{2}{3}$. Expressing it differently, the "cumulant line crossing" is the finite-size effect which should gradually vanish (as $L \rightarrow \infty$) and be replaced by the cumulant-line-splitting picture. This is a consequence of the fact that the low-temperature phase of the two-dimensional XY model is always critical, without having a spontaneous magnetization.

A similar analysis of a variation of cumulants U_L

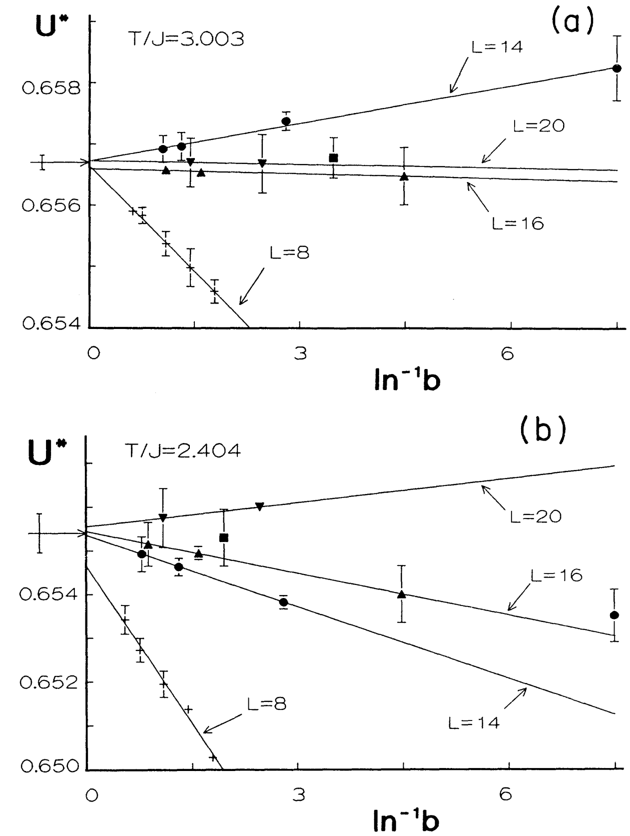

FIG. 3. Estimates for U^* plotted vs inverse logarithm of scale factor b for (a) $T/J=3.003$, and (b) $T/J=2.404$.

$(8 \le L \le 50)$, with J_s/J at $T/J=3.003$, shows that linear fits to the data at $J_s/J \simeq J_s^*/J$ (thin lines) do not have a single intersection, but rather a family of points can be found. Each set is labeled by a lattice size L, the cumulant line of which is crossed by cumulants $U_{L'}$ such that $L'>L$. Also, here, the extrapolation procedure is necessary because of the presence of finite-size corrections to scaling (Fig. 4).

Repeating this procedure for all four temperatures, we arrived at four values of the critical coupling ratios J_s^*/J, which fix positions of four points on the phase boundary

TABLE I. The calculated coordinates of four critical points lying on the surface transition boundary, along with the corresponding values of the fixed-point cumulant. The final estimate of U^* is denoted by U^*_{KT}.

T/J	J_{sc}/J[a]	U^{*b}
2.304	2.107(9)	0.6543(10)
2.404	2.300(4)	0.6554(5)
2.5	2.460(4)	0.6562(2)
3.003	3.113(5)	0.6566(5)

[a] $J_{sm}/J \simeq 1.50(10)$.
[b] $U^*_{\mathrm{KT}} \simeq 0.655(2)$.

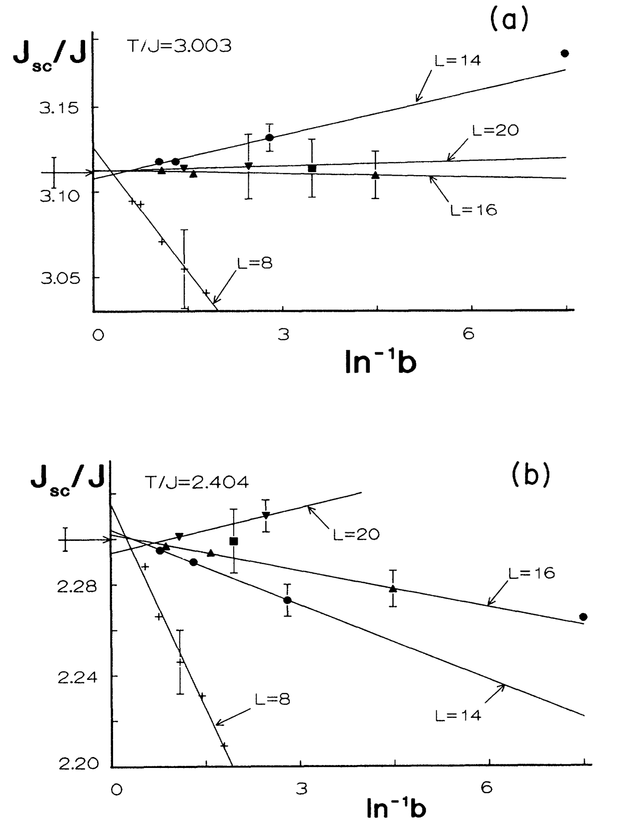

FIG. 4. Estimates for J_s^*/J plotted vs inverse logarithm of scale factor b for (a) $T/J=3.003$, and (b) $T/J=2.404$.

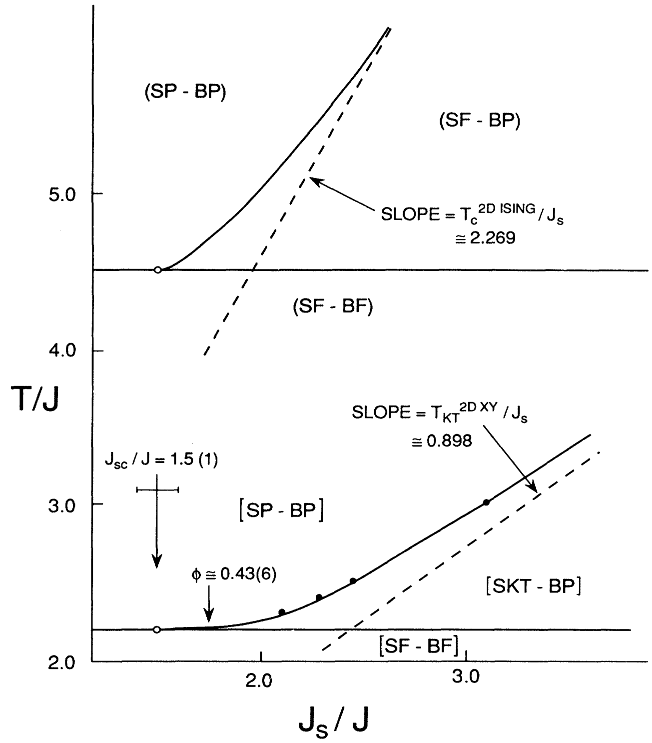

FIG. 5. Phase diagram for the simple cubic (Ref. 4) and the XY (this work) models with modified surface exchange J_s/J plotted on the same scale. The various phases are denoted by round and square brackets (Ising and XY models, respectively) and labeled by bulk (B) and surface (S) properties as ferromagnetic (F), Kosterlitz-Thouless type (KT), or paramagnetic (P). The position of the multicritical point is indicated by an arrow with an error bar ($J_{sc}/J=1.50\pm0.10$).

(Fig. 5). In spite of very small error bars, we do not see the expected merging of the surface transition boundary with its asymptote in the limit $J_s^*/J \gg 1$ (corresponding to decoupling of the surface from the bulk). It is somewhat surprising, particularly if one compares this effect with the case of the Ising model,[4] where a similar merging already takes place for $J_s^*/J \simeq 4$ (Fig. 5). We offer here an explanation using results of a recent study of the 3D layered clock model (in which classical spins interact with nearest neighbors in planes via coupling J_{xy}, which is different than interplanar coupling J_z). Chui and Giri found[29] that in the limit $J_{xy}/J_z \gg 1$ the transition temperature does not extrapolate to T_{KT}, but to a slightly higher value. They explained this effect as being due to the finite thickness of the sample. In order to observe a true asymptotic regime, one would have to study systems with $J_{xy}/J_z > D^2$, D being the transverse dimension of the sample. In our model this would correspond to value of $J_s/J \gg 100$, which was far beyond the scope of our study. It looks then as if the pure planar behavior would be difficult to see, not only experimentally in quasi-two-dimensional magnetic systems[9,17,30,31] (because of an unusually strong crossover to three-dimensional behavior), but in simulational studies as well.[29,32]

The above-mentioned crossover scaling in the surface decoupling limit can, in principle, be described with use of the surface magnetization cumulants data. In the limit $J_s/J \gg 1$, we assume the following crossover scaling *ansatz*:[33]

$$U_L(\xi,(J_s/J),L) \simeq \tilde{U}_L(\xi(J_s/J)^{1/\bar{\varphi}},\xi/L) , \tag{10}$$

which, for $\xi \gg L$, reduces to the form

$$U_L \simeq \hat{U}_L(L(J_s/J)^{1/\bar{\varphi}}) . \tag{11}$$

This implies, for the crossover exponent $\bar{\varphi}$, the following formula:

$$\bar{\varphi} = \frac{\ln(\partial U_{bL}/\partial U_L)_{U^*}}{\ln b} . \tag{12}$$

Since the limit $J_s/J \gg 1$ corresponds to $T/J \gg T_{cb}/J$ ($T_{cb}/J=2.203$ is the bulk critical temperature[34]), one would expect to obtain from the cumulant data taken at $T/J=3.003$ the exponent $\bar{\varphi}$ close to its true, asymptotic value. Unfortunately, the graphical determination of the logarithmic derivative in Eq. (12) demands even more accurate data than those which we obtained: A small change of the slope of linear fit to the data close to the critical point (i.e., close to the intersection with the line of slope 1) gives very different results, so that any further correction to scaling analysis (as described above) is impossible. Our rough estimate $\bar{\varphi}\simeq 0.3\pm 0.2$ can be only qualitatively compared[33] with the value of the crossover exponent for a layered XY model, calculated earlier by Kosterlitz and Thouless[30] and by Hikami and Tsuneto:[35] $\bar{\varphi}\simeq 0.5$.

A line of the surface transition boundary merges with a line of the ordinary transition at the multicritical point with coordinates ($J_s/J\equiv J_{sc}/J$ and $T_c/J=T_{cb}/J$), the position of which can, in principle, be determined using a different crossover scaling analysis. This has been demonstrated for an Ising system by Binder and Landau.[4] There are, however, two important differences in the implementation of this method in a case of the planar rotator model. First, the surface magnetization data cannot be used directly for the purpose of scaling analysis, since m_1 vanishes identically (in the limit of the infinite lattice size) everywhere in the region of phase diagram above the line of the ordinary (and extraordinary) transition. However, the local susceptibility, $\chi_{11}\equiv\partial m_1/\partial h_1$, can be used instead of m_1. Second, the conventional form of the crossover scaling[4,14,36] has to be modified, since the meaningful quantity for the XY-like system is not the reduced temperature but rather the correlation length.[9,30] The local susceptibility χ_{11} for J_s/J near the multicritical point at J_{sc}/J should then depend on the following combination of two variables (T/T_c-1) and $(J_s/J_{sc}-1)$:[14,37]

$$\chi_{11}/[a_\xi\exp(-b_\xi t^{-\bar{\nu}})]^{\bar{\gamma}_{11}^m}=\bar{\chi}_{11}^{sc}(t\Delta^{-1/\phi}) , \tag{13}$$

where $t\equiv T/T_c-1$, $\Delta\equiv J_s/J_{sc}-1$, $\bar{\chi}_{11}^{sc}$ is the appropriate scaling function, and $\bar{\gamma}_{11}^m$ is the value of the local susceptibility exponent at the multicritical point. The above expression implies that, instead of the scaling variables suggested by a conventional scaling of

$$\chi_{11}t^{\gamma_m} \text{ versus } \Delta t^{-\phi} , \tag{14}$$

one should use modified ones:

$$\ln\chi_{11}-(\bar{\gamma}_{11}^m b_\xi)t^{-\bar{\nu}} \text{ versus } \Delta t^{-\phi} . \tag{15}$$

Figure 6 shows the results of an analysis of this type; the data correspond to films with surface size 30×30. As can be seen, the data fall on the universal curve in a quite smooth fashion, using the value of $J_{sc}/J=1.50$; the other parameters were $b_\xi\bar{\gamma}_{11}^m\simeq 0.11\pm 0.02$, and $\phi\simeq 0.43\pm 0.02$. However, a high quality of the fit could be also preserved for all J_{sc}/J in the range 1.40–1.60, where the parameters $b_\xi\bar{\gamma}_{11}^m$ and ϕ varied in the range 0.13–0.10 and 0.39–0.49, respectively.

The self-consistency of the analysis demands[4] that the crossover coefficient ϕ and J_{sc}/J are to be determined by the condition $\bar{\chi}_{11}^{sc}(x_c)=0$, x_c being the scaling variable at the multicritical point: $x_c=t_c\Delta_c^{-1/\phi}$ (where $\Delta_c\equiv J_s^*/J_{sc}-1$, and $t_c\equiv T_s^*/T_c-1$). Then, the exponent ϕ can be determined from the slope of linear fit Δ_c versus t_c. The insert on Fig. 6 shows that the anticipated linear dependence is fairly good (especially for the data in the vicinity of the multicritical point), and that the obtained value of the exponent $\phi=0.42\pm 0.02$ is consistent with the result of scaling of $\bar{\chi}_{11}^{sc}$. However, we suspect that the surface of size 30×30 was too small for the crossover

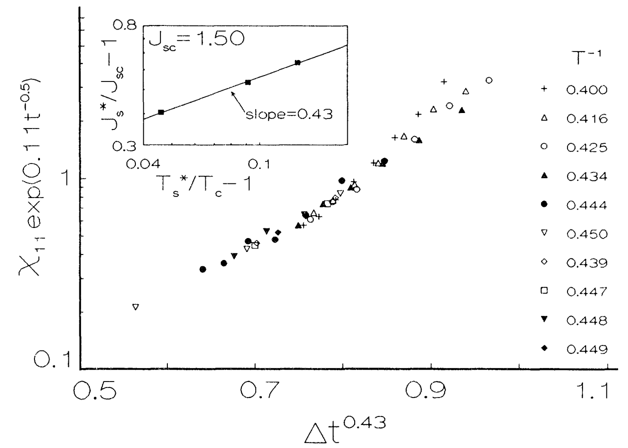

FIG. 6. Scaled local susceptibility $\chi_{11}\exp[(\bar{\gamma}_{11}^m b_\xi)(T/T_m-1)^{-\bar{\nu}}]$ plotted vs the scaling variable $(J_s/J_{sc}-1)(T/T_m-1)^{-\phi}$, for $J_{sc}/J=1.50$, $(\bar{\gamma}_{11}^m b_\xi)=0.11$, and $\phi=0.435$ (the curve refers to $J_s>J_{sc}$). The inset shows the plot of the logarithm of the difference between surface critical coupling J_s^*/J and the multicritical coupling J_{sc}/J vs T_s^*/T_c-1, with the assumption that $J_{sc}/J=1.50\pm 0.10$.

scaling formula, Eq. (13), to be exact (so that additional corrections to scaling would be necessary). Thus the final position of the multicritical point we determined has a rather large error: $J_{sc}/J=1.50\pm 0.10$.

It was impossible in the framework of our analysis to determine an exponent $\bar{\gamma}_{11}^m$ independently of the parameter b_ξ. Since the problem of the measurement of the surface correlation length (i.e., parameters a_ξ and b_ξ) was left out of our study, we can only assume that b_ξ is of the order of the analogous quantity calculated in recent studies of the two-dimensional XY model:[16] $b_\xi\simeq 1.67$, which gives $\bar{\gamma}_{11}^m\simeq 0.066$.

It is also interesting to compare the results of the above analysis with the one carried out with the use of a conventional scaling. Many numerical simulations of the XY model have questioned not only the mechanism behind the Kosterlitz-Thouless transition, but even its order.[18–20,38] In our study we have found a strong evidence against an algebraic-type singularity in this model. Using the conventional scaling variables, we arrived at a fairly good scaling function that was not, however, as smooth as the one obtained with the use of the Kosterlitz-Thouless type of scaling (Fig. 7). Furthermore, this scaling was also consistent with $J_{sc}/J\simeq 1.50$ (± 0.15), $\phi\simeq 0.43$ (± 0.05), and now $\gamma_m\simeq 0.33$ (± 0.05).

Finally, we would like to comment on yet another possibility for crossover scaling that would be also consistent with the Kosterlitz-Thouless type of the surface transition. One could express the local susceptibility χ_{11} in vicinity of J_{sc}/J in terms of the variables t and Δ via

$$\chi_{11}/[a_\xi\exp(-b_x t^{-\bar{\nu}})]^{\bar{\gamma}_{11}^m}=\bar{\chi}_{11}^{sc}[a_\xi\exp(-b_\xi t^{-\bar{\nu}})\Delta^{1/\bar{\phi}}] . \tag{16}$$

Now the corresponding scaling variables should be

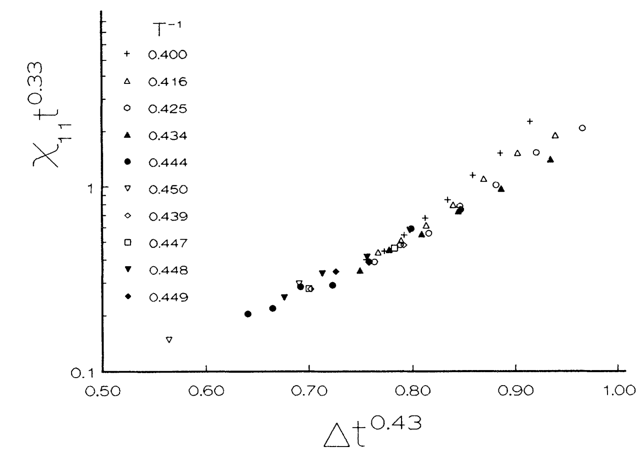

FIG. 7. Scaling of the data in Fig. 6 assuming a power-law divergence of the correlation length [Eq. (14)].

$$\ln\chi_{11}-(\bar{\gamma}^{m}_{11}b_{\xi})t^{-\bar{\nu}} \text{ versus } \ln\Delta+(\bar{\phi}b_{\xi})t^{-\bar{\nu}} . \tag{17}$$

Surprisingly, this type of scaling produced a smooth universe curve and for the same value of $J_{sc}/J \simeq 1.50$ (± 0.15). The other parameters were $b_{\xi}\bar{\gamma}^{m}_{11} \simeq 1.15\pm 0.20$, and $b_{\xi}\bar{\phi} \simeq 0.55\pm 0.14$. The value of the last of the two parameters was consistent with the value obtained from the slope of the linear fit $\ln\Delta_c$ versus $t_c^{-\bar{\nu}}$, although the anticipated linear dependence was only approximate (Fig. 8). This last type of scaling implies, however, that at the multicritical point the line of the surface transitions has an infinite slope, but the size of a region where the inflected boundary would drop down to its terminus would have to be very small, so that the continuation of the boundary (which has a very small slope) would be almost indistinguishable from the appropriate line of slope zero (see the paragraph above). Recent studies of phase diagrams in the $d=3$ semi-infinite anisotropic Heisenberg ferromagnets[39] (the special realization of which includes an isotropic XY model) do not show any indication of this type of anomalies. Thus the above type of crossover scaling does not seem to be appropriate.

B. Surface magnetization

The final part of our study concerns earlier predictions about the nature of the surface transition. We carried out a finite-size-scaling analysis of the surface magnetization m_1, and Fig. 9 shows a logarithmic plot of m_1 versus lattice size L for $T/J=3.003$ (other temperatures show similar results). It is easy to see that the data collected at different regions of phase diagram (i.e., for different values of J_s/J) fall on qualitatively different-looking lines. Whereas the points corresponding to the bulk and surface-disordered phase (BP-SP) lie on a strongly inclined curve, all the data collected in an immediate vicinity of the surface transition and in the bulk-disordered–surface-ordered (BP-SF) region can be fitted with quite high precision to straight lines. This means, that for the whole range of the lattice surfaces investigated, $8 \le L \le 50$, the entire region (BP-SF) is characterized by a power-law behavior of m_1 versus L. But this is a hallmark of the criticality,[9] since there are correlation length is infinite and the corresponding surface order parameter scales like the lattice surface size $L^{-\bar{\beta}}$ [compare Eq. (7)]. Moreover, one can see that each line has a different slope, i.e., the critical exponent $\bar{\beta}$ depends on the position of the point in the Kosterlitz-Thouless phase.

The value of the exponent $\bar{\beta}=\bar{\beta}(J_s^*/J, T/J)$ obtained from the finite-size-scaling analysis (denoted by $\bar{\beta}_{\text{fin}}$) can be compared with results of the analysis of the reduced moments of surface magnetization m_1 (denoted by $\bar{\beta}_{\text{cum}}$).

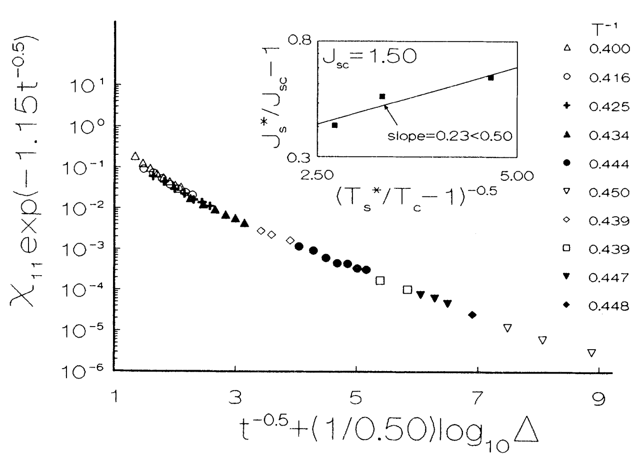

FIG. 8. Scaling of the data in Fig. 6 assuming a full Kosterlitz-Thouless-type divergence of the correlation length [Eq. (17)]. Please note that a logarithmic scale used on a vertical axis spans six orders of magnitude, i.e., three times more than the corresponding axes on Figs. 6 and 7.

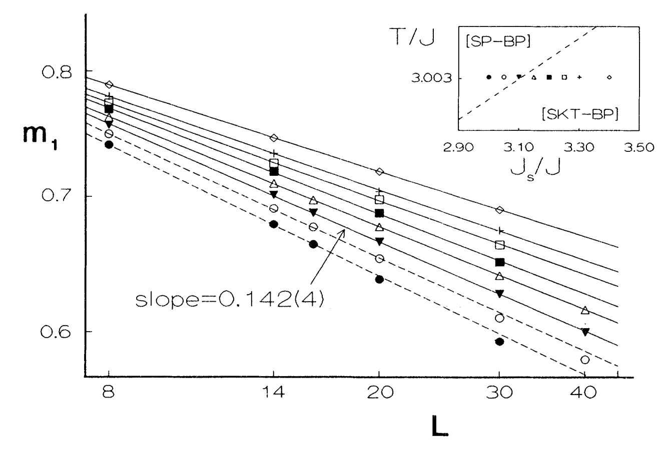

FIG. 9. Log-log plot of the surface magnetization m_1 vs linear dimension of the surface L for $T/J=3.003$ and different values of J_s/J. The dashed lines correspond to the data in the SP-BP region of the phase diagram; the continuous linear fit is possible for the points in the SKT-BP phase (compare the insets in the diagram).

TABLE II. The values of exponents $\bar{\beta}$ obtained from the finite-size-scaling analysis ($\bar{\beta}_{\text{fin}}$) and analysis of the reduced moments of surface magnetization ($\bar{\beta}_{\text{cum}}$). The expected value of $\bar{\beta}$ is denoted as $\bar{\beta}_{\text{exact}}$.

T/J	$\bar{\beta}_{\text{fin}}$	$\bar{\beta}_{\text{cum}}$
2.303	0.146(3)	0.152(3)
2.404	0.144(3)	0.148(4)
2.5	0.143(3)	0.146(2)
3.003	0.139(3)	0.142(3)
	$\bar{\beta}_{\text{exact}}=\eta/2=0.125$	

Because (as we mentioned before) the cumulant type of analysis demands very high-precision data, calculated with the use of the probability distribution moments of the surface magnetization, indices $\bar{\beta}$ have rather large errors; even so the results of the two methods agree very well (Table II). We notice a slight variation of the exponents $\bar{\beta}_{\text{fin}}$ and $\bar{\beta}_{\text{cum}}$ with the temperature, similar to changes found in the analysis of the fixed-point cumulant U^*. Although these changes are marginal, our final estimate of the surface magnetization exponent $\bar{\beta}=0.145\pm0.005$, is rather different from the conjectured value of the exponent $\bar{\beta}=0.125$ ($=\eta/2$), which should be true for any type of the Kosterlitz-Thouless transition.

Similar difficulties in obtaining values of the exponent η (or $\bar{\beta}$) predicted by Kosterlitz were found[16,19,20,22,28] in many other numerical and analytical studies of the 2D XY model. It was suggested[22] that this effect is due to the presence of logarithmic corrections to scaling, similar to those occurring in the XXZ Heisenberg model.[40] If one assumes that these corrections can be represented by the following asymptotic ($L \to \infty$) form of the finite-size scaling of the surface magnetization m_1, so that

$$m_1 \simeq L^{-\bar{\beta}}(\ln L)^{-\bar{x}}, \tag{18}$$

which was found[41] to be correct in case of the $Q=4$ Potts model (which is a special case of the quantum version of the XXZ Hamiltonian[40,42]), then the value of the exponent $\bar{\beta}$, obtained from the slope of the linear fit of $\ln m_1$ versus $\ln L$ corresponding to the KT transition, would be indeed greater then $\eta/2=0.125$. In the framework of this study, we could not, however, determine if this type of correction is valid [one might also consider another multiplicative term in Eq. (18), e.g., $(1+r\ln L)^{-w}$], since the shape of the m_1 versus L line and the values of parameters x, r, and w depend strongly on T/J and J_s/J, i.e., the position of the point $(J_s/J, T/J)$ with respect to the line of the surface transition boundary.

IV. CONCLUSIONS

Using extensive Monte Carlo simulations for films of classical spins, we have studied the surface behavior along the surface transition line and in the vicinity of the multicritical point. We determined the precise position of the boundary between BP-SP and BP-SF phases and demonstrated that the transition is of the Kosterlitz-Thouless type. We could not observe the true asymptotic regime where the surface decoupling takes place, since this effect takes place for very large J_s/J. The finite-size-scaling analysis of the surface magnetization and its probability distribution moments gave us an estimate for the surface magnetization exponent $\bar{\beta}$ associated with the surface transition: $\bar{\beta}=0.145\pm0.005$, which is somewhat larger then the exact value of 0.125. Finally, using crossover scaling, we have determined the approximate position of the multicritical point ($J_{sc}/J=1.50\pm0.10$) and the crossover exponent associated with the special transition: $\phi=0.43\pm0.06$.

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$\bar{\beta}=\eta/2$ (Ref. 9). Since in our model (in the large-system size limit) the magnetization vanishes identically, one should write Eq. (2) with use of the exponent $\eta/2$ rather then $\bar{\beta}$, which we have chosen only because of aesthetic reasons.

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