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Shift of first-order phase transitions in thin films due to boundary fields: A computer simulation

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The first-order phase transition of the ferromagnetic Ising model driven by the magnetic field at temperatures below criticality is studied by Monte Carlo methods for a two-dimensional thin film geometry, $L \times M$ with two free boundaries of length $M \gg L$, at which boundary fields act. This model study is relevant, in particular, for phase transitions in monolayers adsorbed at stepped surfaces. While in the bulk geometry $(L \to \infty)$ this transition occurs for zero field in the present model, with the system "jumping" from a state with uniformly positive magnetization to a state with uniformly negative magnetization, in the thin film geometry the transition occurs at a critical field $H^* \sim L^{-1}$, and the two states between which the transition occurs are characterized by strongly nonuniform magnetization profiles across the film. These findings are in agreement with the scaling theory of Fisher and Nakanishi.

I. INTRODUCTION

There has been a lot of research on surface effects^{1,2} and finite size effects^{3,4} on second-order phase transitions, and the resulting rounding and shifting of critical singularities is fairly well understood. Although first-order phase transitions are even more common in nature than second-order transitions, their rounding and shifting due to finite size has been considered only recently.⁴⁻¹⁴ Most of this work has considered hypercubic L^d systems in d dimensions where moreover surface effects are eliminated by periodic boundary conditions.⁴⁻¹⁰ Then the regions of thermodynamic parameters over which the delta-function singularities are rounded and shifted are of the same order, and fairly small, namely⁴⁻¹⁰ L^{-d} .

The situation is particularly more complicated—and more interesting—when one considers thin film geometries $(L \times M^{d-1}, M \to \infty)^{12-14}$ or long strip geometries $(L^{d-1} \times M, M \to \infty)^{7,11}$ particularly if effects due to free surfaces are included. 12-14 Of course, for the thin film geometry (and assuming discrete broken symmetry of the ordered phase) a sharp first-order phase transition remains: it is then the shift of the transition effected by the finite film width L and/or by "fields" acting at the free boundaries, which is of interest here. While in the long strip geometry the transition is rounded, too, the region over which rounding occurs is predicted to be extremely small, namely¹¹ of the order of $L^{-1/[3(d+1)]} \exp(-\frac{2}{3}L^{d-1}\sigma)$, where σ is the interfacial tension (in units of $k_B T$) between the phases coexisting at the first-order transition. If free surfaces exist with "polarizing" fields (i.e., fields which favor one phase against the other), a shift of order L^{-1} is expected, ¹³ and thus the shift in general is much more important than the rounding, which will not be considered further here for this reason.

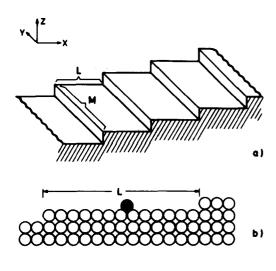
A detailed study of this problem for d = 3 dimensions has been presented by Fisher and Nakanishi, 13,14 with the main intention to understand the criticality of fluids confined between plates. Their analysis is mainly based on scaling considerations and mean-field calculations. We shall summarize their main predictions relevant in the context of our study in Sec. II. Our work rather is concerned with the two-dimensional case which is relevant for first-order transitions occurring in adsorbed monolayers at stepped surfaces (Fig. 1). We have recently analyzed finite-size effects on critical phenomena for such systems. 15,16 Section III briefly characterizes our model and simulation techniques, while Sec. IV presents our results and interprets them in the light of the theoretical predictions. Since the model also displays a second order wetting transition, 16-22 we also pay attention to include the singularity due to the wetting transition into the analysis. Section V summarizes our conclusions.

II. THEORETICAL BACKGROUND

Following Fisher and Nakanishi, 13,14 we consider a ferromagnetic Ising model at temperatures below the bulk critical temperature T_c and study the first-order phase transition observed when the magnetic field H conjugate to the order parameter (the magnetization m) is varied at constant temperature. In the thermodynamic limit, this transition occurs for symmetry reasons at zero magnetic field [Fig. 2(a)], and the states between which the jump of the magnetization occurs are essentially uniform (plus or minus the spontaneous magnetization $m_{\rm sp}$), apart from small local statistical fluctuations (the linear dimension of which is given by the bulk correlation length ξ), as is well known. $^{23-25}$ If we now rather consider an Ising Hamiltonian (H_I) for a thin film (or strip, respectively) of width L with a surface magnetic field acting at its two free boundaries,

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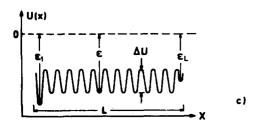


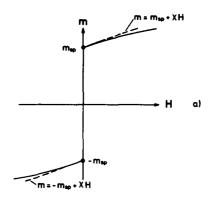
FIG. 1. (a) Schematic view of a regularly stepped surface, where steps a distance L apart in the x direction run parallel to each other a distance M in y direction to form a "stairway" of $L \times M$ terraces, on which adsorption can take place. (b) Cross section through one terrace of width L. Open circles represent substrate atoms, full circle represents an adsorbate atom. (c) Corrugation potential corresponding to the geometry of case (b). We assume that the substrate creates a lattice of preferred sites, at which atoms can be bound to the surface with energy ϵ . In the rows adjacent to the terrace boundaries, however, we assume in general different binding energies ϵ_1 , ϵ_L . The energy barrier ΔU separates neighboring preferred sites.

$$H_{I} = -J \sum_{\langle i,j \rangle} S_{i}S_{j} - H \sum_{i} S_{i}$$

$$-H_{1} \sum_{\substack{k \text{ on boundaries}}} S_{k}, \quad S_{i} = \pm 1, \qquad (1)$$

where an exchange interaction J acts between all pairs $\langle i,j \rangle$ of nearest neighbors on the (square, simple cubic, etc.) lattice, we expect the phase diagram shown qualitatively in Fig. 2(b). Using the well-known²³⁻²⁶ translation from the lattice gas model describing (approximately!) the physical system sketched in Fig. 1, it would be natural to consider a model with two distinct boundary fields H_1 , H_L at the two boundaries^{15,16}; for simplicity we also disregard any possible change of the pairwise interaction J near the boundaries, although models with exchange $J_s \neq J$ in the boundaries can be studied straightforwardly by simulations as well²⁷ and are of interest since the location of the wetting transition then depends on J_s/J .²⁷ Finally we emphasize again that the small rounding¹¹ of the first-order transition in Fig. 2(b) (for d=2), mentioned in the introduction is neglected.

Even for the model Eq. (1) with symmetric boundaries, where consequently magnetization profiles across the strip (Fig. 3) are symmetric around its center, the mean magne-



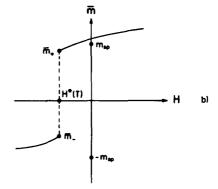


FIG. 2. (a) Schematic plot of the magnetization of an Ising ferromagnet plotted vs magnetic field at a temperature $T < T_c$, for a bulk system where surface effects are negligible. The spontaneous magnetization is denoted as $m_{\rm sp}$, the susceptibility at phase coexistence (H=0) as χ . (b) Schematic plot of the average magnetization \bar{m} of an Ising ferromagnet in a thin film (or strip, respectively) geometry with a positive surface magnetic field H_1 acting on both boundaries. Now the first order transition is shifted from H=0 to a (negative) field $H^*(T)$, and the jump occurs from \bar{m}_+ to $-\bar{m}_-$, where $\bar{m}_+ \neq \bar{m}_- \neq m_{\rm sp}$.

tizations \bar{m}_+ , $|\bar{m}_-|$ characterizing the first-order transition [Fig. 2(b)] are no longer equal. This is obvious, since

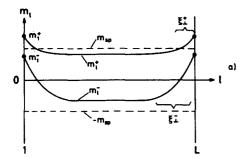
$$\bar{m}_{+} = \left(\frac{1}{L}\right) \sum_{l=1}^{L} m_{l}^{+}, \quad \bar{m}_{-} = \left(\frac{1}{L}\right) \sum_{l=1}^{L} m_{l}^{-},$$
(2)

and for $H_1 \neq 0$ the symmetry $m_l^- = -m_l^+$ is destroyed. Figure 3 emphasizes that there are two lengths ξ_1^+, ξ_1^- describing the two profiles (note that we measure all lengths in units of the lattice spacing). In the nonwet regime of the wetting phase diagram (Fig. 4) far away from the wetting transition both lengths are essentially of the same order as the bulk correlation length ξ . Close to the wetting transition line $H_1(T)$ in the (T,H_1) plane (Fig. 4) the length ξ_1^- in the thermodynamic limit becomes appreciably different from ξ , however. Denoting the distance from the wetting transition line in the (T,H_1) plane by t, correlations between spins are governed by two characteristic lengths ξ_1^-, ξ_1^- (if both spins or only one are located close to the surface), which behave as, 20,28 for d=2 dimensions

$$\xi_{\parallel}^{-}/\xi \sim t^{-\nu_{\parallel}} \tilde{\xi}_{\parallel} \{ t^{-(\nu_{\parallel} + \nu_{\perp})} H \},$$
 (3)

$$\xi_{\perp}^{-}/\xi \sim t^{-\nu_{\perp}} \tilde{\xi}_{\perp} \{ t^{-(\nu_{\parallel} + \nu_{\perp})} H \}$$
 (4)

for a state in the nonwet phase. The scaling functions $\tilde{\xi}_{\parallel}$ and $\tilde{\xi}_{\perp}$ behave such that for $H \neq 0$, $t \rightarrow 0$ the divergence of ξ_{\parallel}^{-} , ξ_{\perp}^{+} is eliminated, which implies



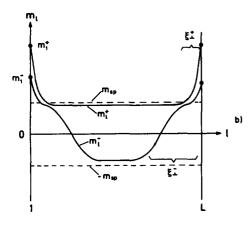


FIG. 3. Schematic plot of the magnetization profiles m_l^+, m_l^- of the strip, characterizing the two states between which the first-order transition shown in Fig. 2(b) occurs. [case (a)] refers to a surface field H_1 which for $L \to \infty$ reduces to "nonwet" magnetization profiles, while case (b) refers to a surface field which for $L \to \infty$ reduces to magnetization profiles in the region of complete wetting. The lengths over which the profile is essentially nonuniform are denoted as ξ_{\perp}^{\pm} .

$$\tilde{\xi}_{\parallel}(z) \sim z^{-\nu_{\parallel}/(\nu_{\parallel}+\nu_{\perp})}, \quad \tilde{\xi}_{\perp}(z) \sim z^{-\nu_{\perp}/(\nu_{\parallel}+\nu_{\perp})},$$
 (5)

and hence for t = 0 simple power laws for $\xi_{\parallel}^-, \xi_{\perp}^-$ are predicted

$$\xi_{\parallel}^{-}/\xi \sim H^{-\nu_{\parallel}/(\nu_{\parallel}+\nu_{\perp})}, \quad \xi_{\perp}^{-}/\xi \sim H^{-\nu_{\perp}/(\nu_{\parallel}+\nu_{\perp})}$$
. (6)

Equation (6) holds also in the wet phase but with different proportionality constants.²⁹ In two dimensions the exponents ν_{\parallel} , ν_{\perp} are believed to be known exactly^{20,21} namely $\nu_{\parallel}=2$, $\nu_{\perp}=1$, and hence Eq. (6) implies $\xi_{\perp}^{-}/\xi_{\sim}H^{-1/3}$. Since the critical field H^* in Fig. 2(b) is of the order $|H^*|\sim 1/L$, as will be discussed below, we conclude that the length ξ_{\perp}^{-} in Fig. 3(b) is of the order $\xi_{\perp}^{-}/\xi_{\sim}L^{1/3}$.

The transverse characteristic length can also be defined in terms of the surface magnetization m_s as

$$\xi_{\perp}^{-}/\xi \sim |m_s^{-}|/m_b \tag{7}$$

with

$$m_s^- = \sum_{l} (m_l^- - m_b)$$
 (8)

and m_b being the magnetization in the bulk ($m_b = \lim_{l \to \infty} \lim_{L \to \infty} m_l$). Alternatively the surface magnetization can be written as the derivative of the surface excess free energy F_s per spin

$$m_s^- = -\left(\frac{\partial F_s^-}{\partial H}\right)_{T,H_1}.$$
 (9)

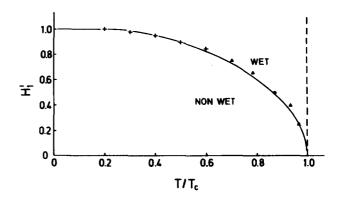


FIG. 4. Phase diagram for the second-order wetting transition of the two-dimensional nearest neighbor square Ising lattice. For fields $H_1 > H_{1c}(T)$ and temperatures $T < T_c$ the boundary of an infinite system with negative spontaneous magnetization is wet while for $H_1 < H_{1c}(T)$ it is nonwet. Full curve is the exact solution of Abraham (Ref. 17) described by the equation $\exp[2J/k_BT]\{\cosh[2J/k_BT] - \cosh[2H_{1c}(T)/k_BT]\}$ = $\sinh[2J/k_BT]$ Points have been found from Monte Carlo calculations on strips of finite width L by various extrapolation procedures, as described elsewhere (Ref. 16).

Since the scaling form for F_s corresponding to Eqs. (3) and (4) is, ²⁸ for d = 2 dimensions

$$F_{s}^{-}(T,H,H_{1}) = F_{s,-}^{\text{reg}}(T,H_{1},H) + t^{\nu_{\parallel}} \widetilde{F}_{s}^{-} \{ t^{-(\nu_{\parallel} + \nu_{\perp})} H \},$$
(10)

where $F_{s,-}^{\text{reg}}$ is a background contribution which is regular at the wetting transition, and \tilde{F} an appropriate scaling function, we conclude from Eqs. (9) and (10)

$$m_{s}^{-} = m_{s}^{\text{reg}} + t^{-\nu_{1}} \tilde{m}_{s}^{-} \{ t^{-(\nu_{\parallel} + \nu_{1})} H \}$$
 (11)

with $m_{s,-}^{\text{reg}} = -\left[\partial F_{s,-}^{\text{reg}}(T,H_1,H)/\partial H\right]_{T,H_1}$, $\tilde{m}_s^-(z) = -\left[\partial \tilde{F}_s^-(z)\right]/(\partial z)$. Equations (7) and (11) again yield Eq. (4).

Now we wish to discuss the location of the critical field $H^*(T)$ where the transition in the bulk of the strip occurs [Fig. 2(b)], considering the limit $L \to \infty$. Then the free energy can be decomposed into bulk and surface terms.

$$F(T,H,H_1,L) = F_b(T,H) + (1/L)F_s(T,H,H_1)$$
. (12)

At a first-order transition two branches of the free energy need to be considered. In the vicinity of the transition both the bulk free energy $F_b\left(T,H\right)$ and the surface correction can be expanded in powers of H,

$$F_{+}(T,H,H_{1},L) = F_{b}(T,0) - m_{sp}H - 1/2\chi H^{2}$$

$$+ 1/LF_{s}^{+}(T,0,H_{1})$$

$$- 1/Lm_{s}^{+}(T,H,H_{1})H \qquad (13a)$$

$$F_{-}(T,H,H_{1},L) = F_{b}(T,0) + m_{sp}H - 1/2\chi H^{2}$$

$$+ 1/LF_{s}^{-}(T,0,H_{1})$$

$$- 1/Lm_{s}^{-}(T,H,H_{1})H. \qquad (13b)$$

Now the transition field $H^*(T,H_1,L)$ simply follows from the condition that the free energies at the two branches are equal,

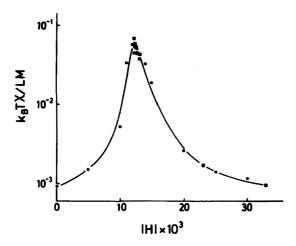


FIG. 5. Susceptibility divided by the volume [Eq. (18)] plotted vs the absolute value of the field, at $T/T_c = 0.95$, $H_1/J = 0.25$, and L = 24, M = 288. Squares denote data obtained from an initial condition {all spins up} while dots from an initial condition {boundary spins up, bulk spins down}. Note that the ordinate scale is logarithmic.

$$F_{+}(T,H^{*},H_{1},L) = F_{-}(T,H^{*},H_{1},L)$$
 which yields

$$H^*(T,H_1,L) = 1/L \left[F_s^+(T,0,H_1) - F_s^-(T,0,H_1) \right] / (\bar{m}_+ - \bar{m}_-) , \quad (15a)$$

$$H^*(T,H_1,L) = 1/L \left[F_s^+(T,0,H_1) \right]$$

$$F_{s}^{-}(T,0,H_{1})]/\{2m_{sp} + (1/L)[m_{s}^{+}(T,H^{*},H_{1}) - m_{s}^{-}(T,H^{*},H_{1})]\}.$$
 (15b)

Thus, we see that to leading order $H^* \sim 1/L$. Since m_s^+ (T,H,H_1) should be regular for $H \to 0$, m_s^+ (T,H^*,H_1) can be replaced by m_s^+ $(T,0,H_1)$ with negligible error. More care is needed with respect to m_s^- , however, due to the singular behavior described by Eq. (11). In the nonwet regime asymptotically for $L \to \infty$, we still may replace $m_s^ (T,H^*,H_1)$ by $m_s^ (T,0,H_1)$. At the wetting transition as well as in the regime of the wet phase, however, we rather have $m_s^ (T,H^*,H_1) \sim H^{*-1/3}$ and putting $H^* \sim 1/L$ this implies $m_s^- \sim L^{1/3}$, yielding a singular correction of order $L^{-2/3}$ to the leading behavior,

$$H^*(T,H_1,L) = [1/(2m_{\rm sp}L)][F_s^+(T,0,H_1) - F_s^-(T,0,H_1)](1 + \text{const } L^{-2/3}).$$
(16)

Finally, we consider the behavior of H^* near the bulk critical temperature T_c : since $m_{\rm sp} \sim (1 - T/T_c)^{\beta}$, $F_s^{\pm}(T,0,H_1) = (1 - T/T_c)^{\gamma} f_s^{\pm}[(1 - T/T_c)^{\Delta_1}, H_1]$ where $\beta = 1/8$, $\nu = 1$, $\Delta_1 = 1/2$ we conclude

$$H^*(T,H_1,L) \sim L^{-1}(1-T/T_c)^{\nu-\beta} \times \{\tilde{f}_s^+ \left[(1-T/T_c)^{-\Delta_1} H_1 \right] - \tilde{f}_s^- \left[(1-T/T_c)^{-\Delta_1} H_1 \right] \}$$
 (17a)

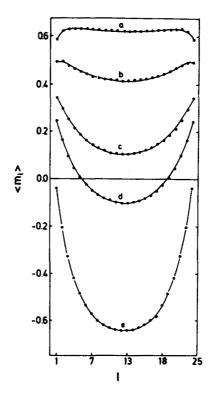


FIG. 6. Magnetization profiles for the nearest neighbor Ising lattice with L=24, M=288 at $T/T_c=0.95$, $H_1/J=0.25$. Five values of the magnetic field are shown: H/J=-0.011(a), -0.0120(b), -0.01249(c), -0.01250(d),

and -0.0140(e). Curves (c) or (d), respectively, correspond to the phase transition, where the maximum of χ occurs, see Fig. 5.

which for small H_1 can be further written [since $\tilde{f}_s^+(0) = \tilde{f}_s^-(0)$]

$$H^{*}(T,H_{1},L) \sim L^{-1}H_{1}(1-T/T_{c})^{\nu-\beta-\Delta_{1}}$$

$$= L^{-1}H_{1}(1-T/T_{c})^{\beta_{1}-\beta}, \qquad (17b)$$

where β_1 is the exponent of the surface layer magnetization $[m_1 \sim (1 - T/T_c)^{\beta_1}]$ with $\beta_1 = 1/2$ here].

Although the present analysis follows the spirit of the discussion of Fisher and Nakanishi, 13,14 an important distinction is that we do not use the mean field theory of critical wetting as done in Refs. 13 and 14, which is clearly not appropriate for our two-dimensional strips, but rather we incorporate the proper scaling theory²⁸ and exponents²⁰ for this case.

III. SOME COMMENTS ON THE SIMULATION TECHNIQUE

We study the Hamiltonian of Eq. (1) by standard Monte Carlo simulation methods. $^{30-32}$ Of course, only systems which are finite in all their linear dimensions can be simulated. So we studied $L \times M$ lattices, with $M \gg L$ and applying periodic boundary conditions along the strip. 15,16 The calculations have been carried out on the multitransputer facility of the university of Mainz $^{33-35}$ (see Ref. 15 for comments on the program implementation on this parallel computer). Typically, two types of the initial conditions were used, one initial condition having all spins up, the second one having all spins down in the bulk of system and only the spins in the boundary rows being up (recall that we chose to work always with positive H_1 , namely $H_1/J = 0.5$ or $H_1/J = 0.25$, respectively). Thus, the first initial condition only relaxes to the upper branch in Fig. 2(b), the second one to the lower

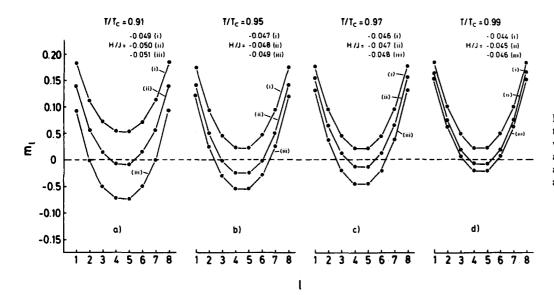


FIG. 7. Magnetization profiles for the nearest neighbor Ising lattice with L=8, M=96, $H_1/J=0.25$ at various temperatures and fields, as indicated in the figure. Curves are only guide to the eye.

branch. For all data the initial 0.25×10^5 Monte Carlo steps (MCS) site were discarded for equilibration and then averages over 1.25×10^5 MCs were taken. Full equilibration is best checked by studying the susceptibility χ defined as

$$k_B T \chi(LM) \equiv \left\langle \left(\sum_i S_i\right)^2 \right\rangle - \left\langle \left(\sum_i S_i\right) \right\rangle^2.$$
 (18)

Figure 5 shows that a unique peak is obtained, with the values of χ being independent of the initial condition, if the system is fully equilibrated. The sharp peak of χ at the transition field H^* in Fig. 5 means that the system jumps back and forth between the two branches in Fig. 2(b), and thus, the observation time sufficiently exceeds the "ergodic time" ³² of the system so that full equilibration actually is achieved.

At a first-order phase transition, of course, γ as defined in Eq. (18) should have a delta-function singularity, and thus Fig. 5 displays clearly a finite-size induced rounding of the transition. Since we work with a finite value of M rather than $M \to \infty$, we do not attempt to analyze this rounding in terms of corresponding theories,11 however. While for $M \rightarrow \infty$ we expect that the strip consists of domains where alternatingly the profiles m_l^-, m_l^+ (Fig. 3) are encountered, separated by walls at a distance $\xi_L \sim L^{1/2} \exp(\sigma L)$, for $M \leqslant \xi_L$ the strip mostly is in a monodomain state. The situation is even more complicated than considered in Ref. 11, since the effective interfacial tension appearing in ξ_L in our case will depend on H_1 . Experience with finite size effects¹⁵ for $H_1 = 0$ suggests that our data fall in a regime, where M and ξ_L are comparable. For the case where $\xi_L \gg M$ the expected description of the rounding is, by a trivial generalization of the arguments of Refs. 7 and 8

$$k_B T \chi_L = k_B T \chi + L M m_{\rm sp}^2 / \cosh^2(L M m_{\rm sp} H / k_B T),$$
(19)

if the deviation of \bar{m}_+ from $m_{\rm sp}$ and \bar{m}_- from $-m_{\rm sp}$ is neglected. However, no analysis of the rounding in the region where ξ_L and M are of the same order is known to us yet.

When we increase L (and/or decrease T) pronounced hysteresis effects occur, since then the ergodic time of the model is already larger than the chosen observation time. Thus, the largest systems simulated were L=72, M=864 ($T/T_c=0.99$) and L=36, M=432 ($T/T_c=0.95$), since then the width ΔH^* of the field region over which hysteresis occurs was very small.

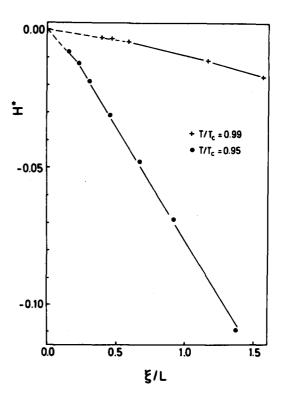


FIG. 8. Plot of H^* vs ξ/L for $T/T_c = 0.99$ (crosses) and $T/T_c = 0.95$ (dots). Note that $\xi(T/T_c = 0.99) \approx 28.162$ and $\xi(T/T_c = 0.95) = 5.476$, using the exact (Ref. 36) results for ξ . All data refer to $H_1/J = 0.25$ and a system shape of M/L = 12. Here H^* is defined as that value of the bulk field at which the magnetization m_l in the center of the film vanishes.

IV. NUMERICAL RESULTS FOR THE MAGNETIZATION PROFILES

In Fig. 6 we present data for the evolution of the magnetization profile as a function of the magnetic field at fixed temperature $T/T_c=0.95$. It is seen that throughout the transition region the magnetization profiles are distinctly nonuniform. The general features of the profile are similar as Fig. 3(a), as expected, since from Fig. 4 we conclude that the considered state belongs to the nonwet region. In view of the fact that there is a slight rounding of the first order transition (Fig. 5) it is difficult to estimate the precise amount of the jump from m_l^+ to m_l^- . Figure 7 shows the temperature evolution of the profile. It is seen that the variation of the profile as a function of H gets smoother as $T \rightarrow T_c$, consistent with the expectation that $\lim_{T \rightarrow T_c(L,H_1)} (m_l^+ - m_l^-) = 0$, where $T_c(L,H_1)$ is the critical point at which the first order phase boundary $H^*(T,L,H_1)$ terminates.

Figure 8 shows the resulting size dependence of the critical field $H^*(T,H_1,L)$ at which the first order phase transition occurs. The predicted behavior $H^*(T,H_1,L) \sim L^{-1}$ is nicely verified. However, the asymptotic region is only reached for $\xi/L \ll 1$. This is not unexpected, in view of the singular corrections [Eq. (16)]. Note that for $T/T_c = 0.95$ ($T/T_c = 0.99$) the data shown in Fig. 8 are in the nonwet (wet) region of the phase diagram for critical wetting, respectively, Fig. 4. A plot of LH^* vs $L^{-2/3}$ for large L is

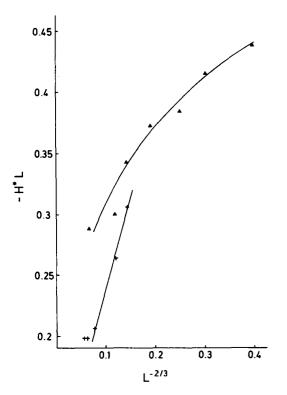


FIG. 9. Plot of H^*L vs $L^{-2/3}$ for $T/T_c=0.95$ (triangles) and $T/T_c=0.99$ (crosses). The straight line tentatively illustrates Eq. (16). Note that the state for $T/T_c=0.95$ is in the nonwet region, where Eq. (16) does not hold, but rather an analytic dependence of H^*L on L^{-1} is expected. Curve through these data is a guide to the eye only.

roughly consistent with Eq. (16), see Fig. 9, although the scatter of the data points is too large to actually "prove" Eq. (16) convincingly.

V. CONCLUSIONS

In this paper we have considered the shift of first order phase transitions in strips of finite width L, by carrying out both a phenomenological scaling analysis and Monte Carlo simulations for a nearest-neighbor Ising (or lattice gas) model. It is shown that to leading order the shift is of order L^{-1} , while the next-to-leading order is proportional to $L^{-5/3}$ if the boundary wets the strip. However, all of our considerations are restricted to the case where the perturbation due to the boundary potential is of strictly short range.

Our simulations thus confirm predictions that have been made first by Fisher and Nakanishi^{13,14} in their pioneering work addressing the critical point shifts of fluids or fluid binary mixtures confined between plates. Since our work is for two-dimensional systems, it is more directly applicable to first-order phase transitions occuring on stepped surfaces, with L being the terrace width between the steps (Fig. 1). Of course, our analysis applies qualitatively only in the case of a linear coupling between the boundary potential and the order parameter distinguishing the phases at the first-order transition.

As is well known, 20 boundary perturbations often are of long range rather than of short range. While the leading behavior $H^*(T) \sim L^{-1}$ presumably stays unaffected, a distinct effect on the leading correction to this behavior depending on the range of the perturbation is expected.

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