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Wetting transitions near the bulk critical point: Monte Carlo simulations for the Ising model

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Critical, tricritical, and first-order wetting transitions are studied near the bulk critical point of a simple cubic nearest-neighbor Ising model by extensive Monte Carlo simulations. The model applies an exchange J in the bulk and exchange J_s in the surface planes, where surface fields H_1 also act in addition to a possible bulk field H. Lattices in a thin-film geometry $L \times L \times D$ are used, with two free $L \times L$ surfaces (with L up to 256) and film thickness D up to 160, applying a very fast fully vectorizing multispin coding program. Our results present the first quantitative evidence for the scaling theory due to Nakanishi and Fisher, which links wetting behavior and surface critical behavior. In particular, we show that the tricritical wetting line (J_s^t/J) merges into the surface-bulk multicritical point with associated critical field $H_{1t} \sim (1-T/T_c)^{\Delta 1m}$, while the critical field for critical wetting H_{1c} vanishes as $H_{1c} \sim (1-T/T_c)^{\Delta_1}$, where $\Delta_1(\Delta_{1m})$ are the "gap" exponents for the surface-layer magnetization at the ordinary (or surface-bulk multicritical) transition. The mean-field character of critical wetting in this model is again confirmed.

I. INTRODUCTION AND OVERVIEW

Wetting phenomena have found much attention recently.[1-4] It has been predicted that both second-order and first-order wetting transitions are possible, although experimental evidence so far is restricted to first-order wetting. However, recent Monte Carlo work[5-9] where wetting phenomena in a nearest-neighbor simple-cubic Ising model induced by a surface magnetic field H_1 have been simulated, has allowed a study of both critical, tricritical, and first-order wetting. Although it is unclear to which extent this very simple model relates to any real materials, these simulations allow us to address several problems of great current theoretical interest: For the problem of critical wetting with short-range forces, renormalization-group theory predicts[10-13] that the exponent $\nu_\parallel$ characterizing the divergence of the correlation length parallel to the surface differs appreciably from the mean-field prediction $\nu_\parallel = 1$. Since the corresponding Monte Carlo studies[7,8] were consistent with $\nu_\parallel = 1$, however, a discussion was initiated in the recent literature concerning the reasons for this discrepancy.[14-17] Of course, for Monte Carlo work one may always raise the possibility that the data were not accurate enough, or that the asymptotic critical region was not reached, etc. Thus, in the Appendix to the present paper we shall reconsider our previous analysis[7,8] and show that significantly better data do not alter our previous conclusions.

The main focus of this paper, however, is the connection between wetting phenomena near a critical point in the bulk and surface critical phenomena, which was suggested by Nakanishi and Fisher[18] (Fig. 1). The prototype model for the understanding of surface critical phenomena[19-22] is a semi-infinite Ising ferromagnet with exchange J_s in the free surface plane different from the exchange J in the bulk, and this model is also considered here. As is well known, three cases (for $J_s > 0$) need to be distinguished depending on the ratio J_s/J: For J_s less than a multicritical value, the surface exhibits the so-called "ordinary transition,"[19,20] i.e., the surface disorders at the same temperature T_c as the bulk does, and the bulk correlation length ξ_b also controls correlation functions near the surface. The new feature of surface criticality not contained in the knowledge of the bulk critical exponents enters when we consider the response to a surface magnetic field H_1, different from the bulk field H. There now exists ample evidence[19-21] for a scaling theory[22-24] which implies that the singular part of the surface excess free energy f_s (per spin) can be written

$$f_s^{\text{sing}}(T,H,H_1) = t^{2-\alpha-\nu}\tilde{f}_s^{\pm}(Ht^{-\Delta}, H_1 t^{-\Delta_1}) , \qquad (1)$$

where $t = |1-T/T_c|$. The two superscripts $\pm$ of the

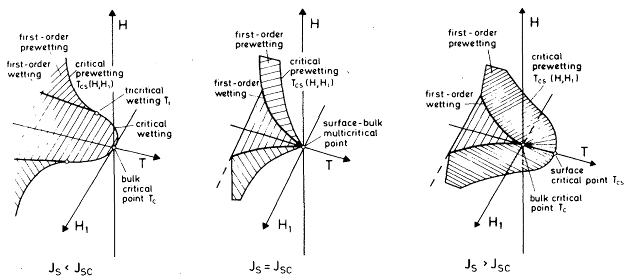

FIG. 1. Schematic phase diagrams of a semi-infinite Ising magnet in the vicinity of the bulk critical point T_c as a function of temperature, bulk field H, and surface field H_1. In the shaded part of the $T-H_1$ plane (i.e., $H=0$) the system for $T<T_c$ is nonwet, while outside of it for $T<T_c$ it is wet. The wetting transition is shown by a thin line where it is second order and by a thick line where it is first order. First-order prewetting surfaces terminate in the plane $H=0$ at the first-order wetting line. For surface exchange J_s less than the surface-bulk multicritical value J_{sc} (left part) there exists a tricritical wetting transition at a temperature $T_t<T_c$, while for $J_s=J_{sc}$, T_t merges with the surface-bulk multicritical point (middle part). For $J_s>J_{sc}$ (right part) only first-order wetting is possible; the surface transition T_{cs} (where for $H=H_1=0$ the surface develops spontaneously two-dimensional order before the bulk) is just a point on the prewetting critical line $T=T_{cs}$ (H,H_1): after Nakanishi and Fisher (Ref. 18).

scaling function $\tilde{f}_s^{\pm}$ refer to $T>T_c$ $(+)$ and $T<T_c(-)$, respectively; α is the bulk specific-heat exponent, ν the correlation length exponent, and Δ the gap exponent. The basic new exponent expressing the surface effects is Δ_1.

In the regime $J_s>J_{sc}$, however, the surface orders spontaneously at a temperature $T_{cs}>T_c$, so the bulk stays disordered. The correlation length for correlations perpendicular to the surface stays finite at this so-called "surface transition," while the correlation length parallel to the surface diverges, the exponent having the standard value ($\nu=1$) for bulk two-dimensional criticality (all other exponents have their standard two-dimensional Ising-model values as well).

These two regimes merge for $J_s=J_{sc}$ at the surface-bulk multicritical point, where $T_{cs}=T_c$ and two- and three-dimensional correlations simultaneously become critical. In the asymptotic vicinity of this point a crossover-scaling generalization of Eq. (1) holds,

$$f_s^{\rm sing}\left[T,H,H_1,\frac{J_s}{J_{sc}}-1\right] =t^{2-\alpha-\nu}\tilde{f}_{s,m}^{\pm}\left[Ht^{-\Delta},H_1t^{-\Delta_{1m}},\left[\frac{J_s}{J_{sc}}-1\right]t^{-\varphi}\right]. \tag{2}$$

Here Δ_{1m} takes a (multicritical) value different from Δ_1 at the ordinary transition and φ is a crossover exponent. Note that the surface transition for $J_s \gtrsim J_{sc}$ is incorporated in this description; it corresponds to a singularity of the scaling function $\tilde{f}_{s,m}^{+}$ (x,y,z) for some value $z=z_c>0$ in the limit $x\to 0$, $y\to 0$.

Now the semi-infinite Ising model with a surface field H_1 competing with the spontaneous magnetization in the bulk is also a prototype model for wetting with short-range forces.[1-8,25] Thus it is rather natural to expect that some relation to surface critical phenomena should exist.[18] Nakanishi and Fisher[18] made this connection more specific, by proposing that the wetting and prewetting transition phenomena near T_c are described by appropriate singularities of the surface excess free energy scaling functions $\tilde{f}_s^{-}$ [Eq. (1)] and $\tilde{f}_{sm}^{\pm}$ [Eq. (2)]. Moreover, they propose a specific *phase diagram topology* (Fig. 1) which incorporates the above scenario of surface critical phenomena as well as critical, tricritical, and first-order wetting transitions, and first- and second-order prewetting. Most intriguing is the prediction that a tricritical wetting transition (and hence a critical wetting line) should exist only for $J_s<J_{sc}$, which implies that the surface-bulk multicritical point is an endpoint of the tricritical wetting line.[18,8]

Although these predictions are plausible and their validity has been widely assumed,[8] previous Monte Carlo work[5-8] was completely unable to test it: Even though system sizes up to 10^5 Ising spins were simulated, both finite-size effects and strong interfacial fluctuations restricted the temperature region that could be investigated to $k_BT/J\le 4$. Since the correlation length in the bulk is already very small there, of the order of a lattice spacing,[26] these data (Refs. 5–8) fall completely outside of the critical region where Eqs. (1) and (2) hold.

This limitation is now overcome in the present paper. Applying a novel vectorizing multispin-coding algorithm[27] in every two-dimensional $L\times L$ plane parallel to the free surface together with the technique of preferential surface site selection,[5-8] the simulation program performs about two orders of magnitude faster (on the CDC Cyber 205 of the University of Georgia) than the conventional program used for the earlier studies[5-8,21] on serial computers. Studying systems in a "thin-film" geometry $L\times L\times D$, with two free $L\times L$ surfaces, we now are able to go to sizes up to $L=256$ and $D=160$, i.e., systems containing several millions of Ising spins. Even such sizes turn out to be just sufficient to enter the critical region far enough to significantly address the problem posed.

Section II now precisely specifies the model and defines the quantities that are analyzed. General considerations about simulations of this type can be found in our earlier work (Ref. 8) and will not be repeated here. Section III presents the data analysis for critical wetting, Sec. IV for tricritical and first-order wetting. The discussion of our results in terms of Eqs. (1) and (2) is presented in the concluding Sec. V. The reinvestigation of critical exponents for critical wetting is deferred to the Appendix.

II. MODEL AND CALCULATED QUANTITIES

We consider simple-cubic Ising $L\times L\times D$ systems with two equivalent free $L\times L$ surfaces and periodic boundary conditions in the two remaining directions. As discussed above, the Hamiltonian is

$$\mathcal{H}=-J\sum_{\text{bulk}}\sigma_i\sigma_j-J_s\sum_{\text{surfaces}}\sigma_i\sigma_j-H\sum_i\sigma_i$$
$$-H_1\sum_{\text{surfaces}}\sigma_j,\quad \sigma_i=\pm 1\ . \tag{3}$$

While the vectorizing multispin-coding program allows maximum efficiency only for $L=64$ or an integer multiple thereof,[27] D is arbitrary. Our standard choice for L is $L=128$, while occasionally $L=64$ and $L=256$ are also used, particularly for ascertaining finite-size effects. While at temperatures far below T_c reasonable results can be obtained[5–8] using $D=40$, we must use considerably thicker films ($D=80$ and $D=160$, respectively), closer to T_c. Such thick films are necessary to maintain the metastable configuration of a film with positive magnetization in the bulk for negative surface field H_1 and $H=0$ for sufficiently long observation times, as discussed in Ref. 8.

Among the quantities which are recorded are the profiles of magnetization m_n and energy U_n (n is the layer index which runs from 1 to D, where the lattice spacing is equal to unity). We also record a bulk magnetization m_b and energy U_b defined from an average over the 20 innermost layers. These quantities are compared to estimates of m_b, U_b from independent runs for systems without free surfaces, to check that the system in the bulk is not affected by the free surfaces and the wetting layers possibly attached to them, and thus we learn whether D has been chosen large enough.

From the layer quantities we can also obtain the surface excess magnetization m_s and surface excess energy U_s as follows:[19–22]

$$2m_s=\sum_{n=1}^{D}(m_b-m_n)\ ,$$
$$2U_s=\sum_{n=1}^{D}(U_b-U_n)\ . \tag{4}$$

Note that the factor 2 simply comes from the fact that we have two free surfaces.

A further quantity on which we focus here is the surface layer susceptibility χ_1 defined by[19–22]

$$\chi_1=\left[\frac{\partial m_1}{\partial H}\right]_T=-\left[\frac{\partial^2 f_s}{\partial H\partial H_1}\right]_T, \tag{5}$$

which we calculate using the fluctuation relation

$$k_BT\chi_1=L^2D\left[\left\langle\frac{1}{2L^2}\sum_{\text{surfaces}}\sigma_k\frac{1}{L^2D}\sum_i\sigma_i\right\rangle-\left\langle\frac{1}{2L^2}\sum_{\text{surfaces}}\sigma_k\right\rangle\left\langle\frac{1}{L^2D}\sum_i\sigma_i\right\rangle\right]. \tag{6}$$

Temperatures studied include $J/k_BT=0.230$, 0.226, and 0.224 (note that bulk criticality occurs for[28] $J/k_BT\approx 0.2217$, and thus we approach to within 1% of the critical point); in some cases data obtained for smaller sizes ($L=30$ and 50, and $D=40$, respectively), from the previous investigation[8] are included. The exponents of critical wetting, however, are studied far below T_c at $J/k_BT=0.35$, in order to reduce fluctuations in the bulk.

III. CRITICAL WETTING

As was previously[5–8] discussed we concentrate on $J_s=J$ and scan the surface field H_1, trying to locate the critical wetting transition from the maximum of χ_1 and the behavior of the surface excess quantities (Figs. 2–5): Recall that both mean-field and renormalization-group theories imply a Curie-Weiss-type divergence of χ_1 as the wetting transition is approached from the nonwet side,[1,2]

$$\chi_1\sim(H_1-H_{1c})^{-1}\ , \tag{7}$$

while the surface excess magnetization should show a logarithmic divergence,

$$m_s\sim-\ln(H_1-H_{1c})\ . \tag{8}$$

The surface excess energy U_s is expected to show a rounded peak near H_{1c}, and can be used to locate H_{1c} only rather roughly.

Figures 2 and 3 show that even for the temperature $J/k_BT=0.23$, which is rather far away from T_c

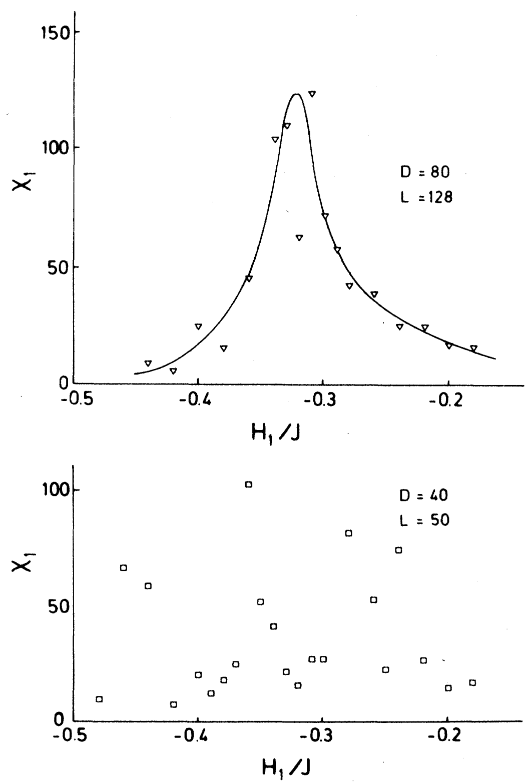

FIG. 2. Surface-layer susceptibility χ_1 at $J/k_BT=0.23$ and $J_s=J$ plotted vs surface field. Lower part shows data for a $50\times50\times40$ system, upper part shows data for a $128\times128\times80$ system. Curve in the upper part is only a guide to the eye.

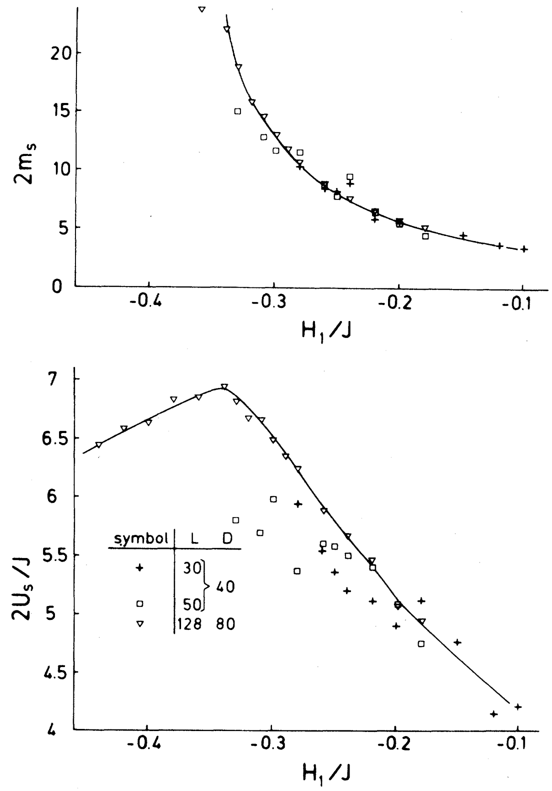

FIG. 3. Surface excess magnetization (upper part) and surface excess energy (lower part) plotted vs surface field for $J/k_BT=0.23$ and $J_s=J$. Several system sizes are included as indicated. Curves through the data points of the largest systems are guides to the eye only.

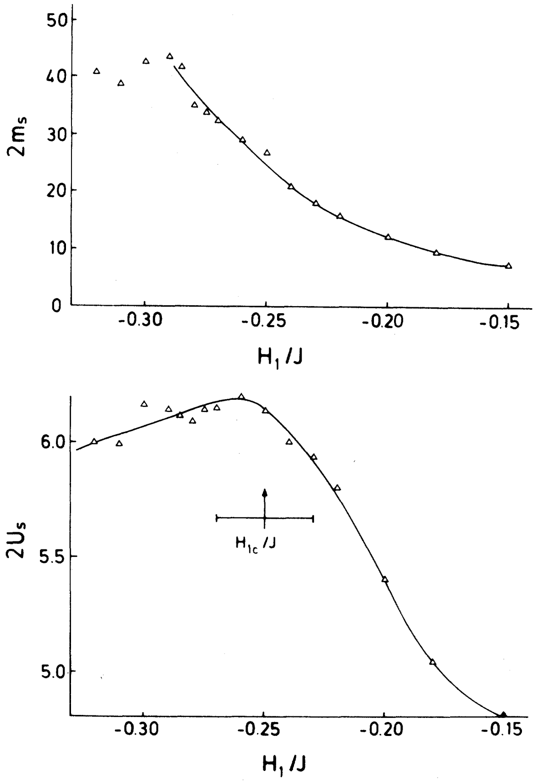

FIG. 4. Surface excess magnetization (upper part) and surface excess energy (lower part) plotted vs surface field for $J/k_BT=0.226$, $J_s=J$, and a $128\times128\times160$ system.

($\xi_b\approx2.01$), the data from the $30\times30\times40$ and $50\times50\times40$ systems are too noisy to allow any useful analysis. The availability of large systems is absolutely crucial for the present study—only then is the system sufficiently metastable to allow statistically meaningful "measurements." The accuracy of the small system data cannot be improved by increasing the observation time: What happens is that the two interfaces between up and down phases near the walls fluctuate so strongly that they meet and overturn the whole film, which then remains in this stable state (i.e., magnetization in the bulk being parallel to the surface field). For the large system, self-averaging quantities[29,30] like m_s and U_s have very satisfactory accuracy (Fig. 3), while χ_1, which is obtained from sampling fluctuations [Eq. (6)] and hence is not self-averaging,[29,30] shows appreciable scatter even for the large system (Fig. 2). The improvement in accuracy in the upper part of Fig. 2 simply is due to the fact that a much larger number of statistically independent configurations could be generated for the larger system, first of all because the program used is so much faster, and second because the system is sufficiently metastable. Thus from Fig. 2, upper part, we may conclude that $H_{1c}/J=-0.325\pm0.015$, and this estimate is compatible with Fig. 3. Of course, this accuracy in locating a critical wetting transition is not really impressive—but in order to improve it significantly, much larger systems need to be simulated for much longer times, which is beyond the possibilities of presently available computers.

In view of these difficulties, it is no surprise that the situation is worse for $J/k_BT=0.226$ (where $\xi_b\approx3.08$ and

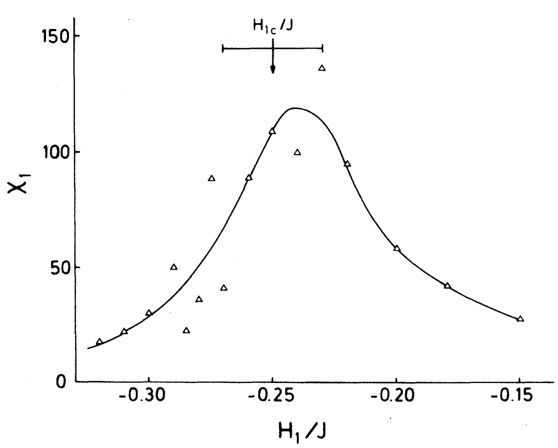

FIG. 5. Surface-layer susceptibility χ_1 plotted vs surface field for $J/k_BT=0.226$, $J_s=J$, and a $128\times128\times160$ system.

hence the *effective* system size—if we rescale both L and D with ξ_b—would be significantly smaller). Now U_s and m_s already exhibit considerable fluctuations, see Fig. 4—although most of the data points are averages over 4 independent runs taking a CPU time of about 40 minutes each,[31] while Figs. 2 and 3 show data from single runs of the same length. Thus, we end up with an estimate of $H_{1c}/J \approx -0.25 \pm 0.02$. The relative error is now about twice as large as for $J/k_BT=0.23$, in spite of the considerably larger statistical effort. In view of these problems, we have not attempted to go closer to T_c for $J_s/J=1$.

IV. FIRST-ORDER WETTING AND TRICRITICAL WETTING

Locating a first-order wetting transition is somewhat simpler than locating a second-order wetting transition, since first-order wetting shows up via a distinct jump in the magnetization m_1 of the first layer (Fig. 6). This jump leads to a value of m_1 in the wet phase which is more negative than the negative value of the bulk magnetization. As the ratio J_s/J decreases, the jump of m_1 also decreases and vanishes at the wetting tricritical point J_{st}. Of course, one again has to worry about the accuracy of the estimates for J_{st} and the associated tricritical field H_t due to finite-size effects and limited observation time; since, in practice, the range of J_s/J values and fields H_t where the tricritical point probably is located, is rather small, we can obtain a reasonable accuracy for both $J/k_BT=0.23$, 0.226, and 0.224. Thus, we estimate $J_{st}/J=1.29\pm0.01$, $H_{1t}/J=-0.130\pm0.002$ $(J/k_BT=0.23)$, $J_{st}/J=1.33\pm0.01$, $H_{1t}/J=-0.074\pm0.002$ $(J/k_BT=0.226)$, and $J_{st}/J=1.41\pm0.01$, $H_{1t}/J=-0.035\pm0.005$ $(J/k_BT=0.224)$. Again, the availability of very large systems turns out to be extremely crucial for the feasibility of this study—this is obvious from the fact that the magnetization profile m_n develops a significant variation over up to 40 layers near the surface, when one approaches the tricritical wetting transition from the nonwet side (Fig. 7) and from the fact that pronounced and nontrivial finite-size effects are present (Figs. 8 and 9). Note that Eqs. (7) and (8) hold for a tricritical wetting transition as well,[1,2] and the data in Figs.

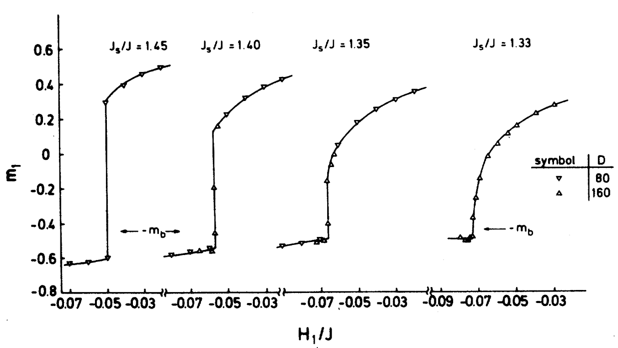

FIG. 6. Surface-layer magnetization m_1 plotted vs surface field for $J/k_BT=0.226$ and several values of J_s/J. Data are for $L=128$ and two values of D, as indicated in the figure.

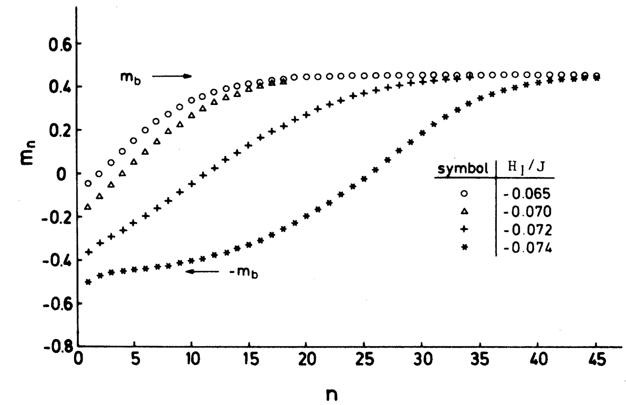

FIG. 7. Magnetization profiles (layer magnetization m_n plotted vs layer number n) for $J/k_BT=0.226$, $J_s/J=1.33$, a $128\times128\times160$ system, and several values of the surface field. Note that within our accuracy $H_1/J=-0.074$ is the tricritical field.

8 and 9 are consistent with this. It would be interesting to analyze the finite-size effects more quantitatively and compare them with current theories[32] on finite-size scaling for wetting transitions—unfortunately the large scatter of the data in Figs. 8 and 9 prevents us from doing so. This problem would at best be tractable at rather low temperatures, outside the regime of interest of the present work.

V. EVIDENCE FOR THE CONNECTIONS BETWEEN WETTING AND SURFACE CRITICAL PHENOMENA

We now turn to the question of to what extent our data prove or disprove the scenario of Nakanishi and Fisher,[18] as described in Sec. I and sketched in Fig. 1. First of all, we consider the question of whether the surface-bulk multicritical point[19–23] (which for the simple-cubic

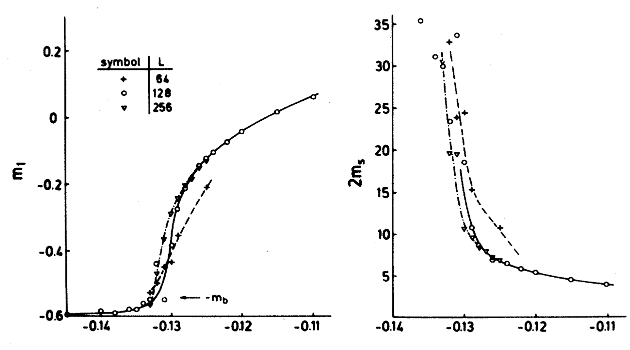

FIG. 8. Surface-layer magnetization m_1 (left part) and surface excess magnetization m_s (right part) plotted vs surface field for $J/k_BT=0.230$, $J_s/J=1.28$, and $D=80$, for three values of L. Note that within our accuracy this choice of parameters corresponds to a tricritical wetting situation. All curves are only guides to the eye.

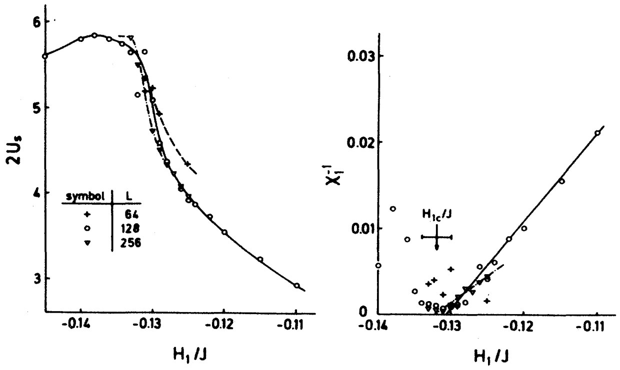

FIG. 9. Surface excess energy (left part) and inverse surface-layer susceptibility χ_1^{-1} (right part) plotted vs surface field, for the same parameters as in Fig. 8.

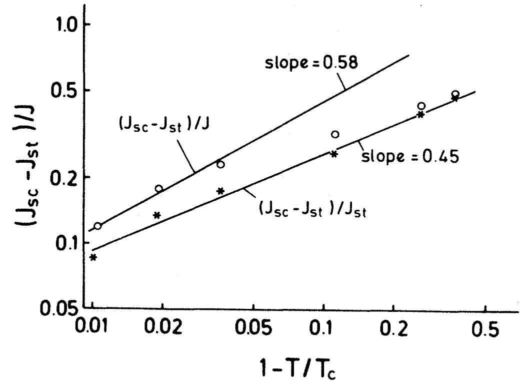

FIG. 11. Log-log plot of $(J_{sc}-J_{st})/J$ (dots) and $(J_{sc}-J_{st})/J_{st}$ (crosses) vs $1-T/T_c$. Straight lines show possible effective exponents fitted to these data in different temperature regimes.

nearest-neighbor Ising model occurs for[21] $J_{sc}/J \approx 1.52 \pm 0.01$) is actually the endpoint of the line of tricritical wetting transition J_{st}/J in the plane of variables J_s/J and J/k_BT. Figure 10 shows that our data are, in fact, nicely consistent with this conjecture, and in addition imply that the curve $J_{st}(T)/J$ merges at T_c into J_{sc}/J with infinite slope. For lower temperatures the curve of tricritical wetting transitions must end at the roughening transition, where wetting phenomena get replaced by layering.[25] The roughening temperature is estimated as[33] $J/k_BT_R \approx 0.41$. Some preliminary evidence for layering at $T<T_R$ has already been presented,[8] and a more detailed analysis is planned to be presented elsewhere.[34]

Now Eq. (2), which implies that tricritical wetting is a singularity of the scaling function $\tilde{f}_{s,m}^{-}$ $(x=0,y,z)$ at $z=z_t$, yields a quantitative prediction for the tricritical wetting curve near J_{sc}: The equation $z=z_t$ for $J_s=J_{st}$ implies

$$\frac{J_{st}}{J_{sc}}-1 \sim |1-T/T_c|^{\varphi} . \tag{9}$$

Figure 11 tests this relation by a log-log plot. Only the data closest to T_c are consistent with the suggested value[21] $\varphi \approx 0.58$. The data could be fitted over a much larger range of temperatures to a significantly smaller effective exponent $\varphi \approx 0.45$. However, this observation may be just a consequence of corrections to scaling—in

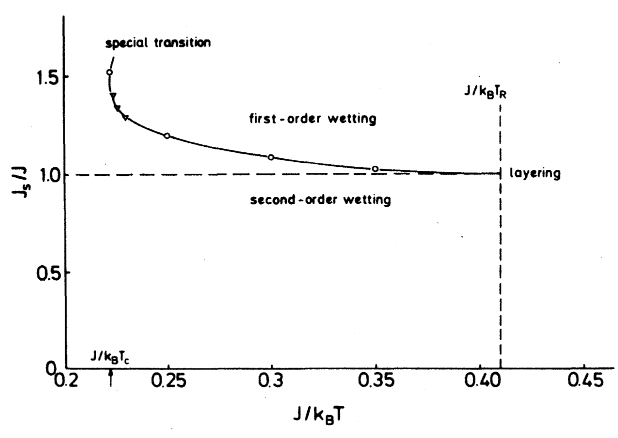

FIG. 10. Surface phase diagram, in the plane of variables J_s/J and J/k_BT, exhibiting the line of tricritical wetting transitions, separating the region of first-order wetting (above this line) from second-order wetting (below this line). The tricritical wetting line at J/k_BT_c ends in the so-called "special transition" (or surface-bulk multicritical point), and at lower temperatures it ends at the roughening temperature, where layering transitions replace wetting (Ref. 25). The estimate for T_R was taken from Mon *et al.* (Ref. 33).

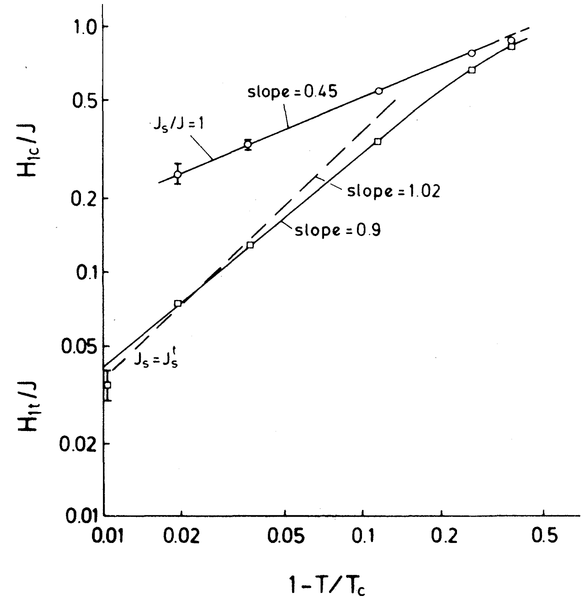

FIG. 12. Log-log plot of the temperature dependence of the critical field H_{1c} at the critical wetting transition for $J_s/J=1$ (upper part) and at the tricritical wetting transition (lower part). Dashed and solid straight lines show possible effective exponents extracted from these data.

fact, somewhat different exponents are already seen when $(J_{sc}-J_{st})/J_{st}$ instead of $(J_{sc}-J_{st})/J$ is plotted (Fig. 11).

Figure 12 shows that we are more successful with respect to the variation of the critical fields H_{1c} and H_{1t}. Equation (1) implies that critical wetting is a singularity of the scaling function $\tilde{f}_s^-(x=0,y=y_c)$, i.e., H_{1c} should vanish near T_c as $H_{1c}\sim(1-T/T_c)^{\Delta_1}$, and at the tricritical transition H_{1t} we should have $H_{1t}\sim(1-T/T_c)^{\Delta_{1m}}$. The data (Fig. 12) not only are compatible with such power laws, but the exponent estimates resulting from Fig. 12, namely, $\Delta_1=0.45$, $\Delta_{1m}\approx 1.02$, are also within their errors (the relative error is at least 5% in both cases) in full agreement with the expected values.[21] All together the data presented in Figs. 10–12 provide satisfactory evidence that the hypothesis of Nakanishi and Fisher[18] relating wetting and surface critical phenomena is valid.

Of course, it would be desirable to approach the bulk critical point still closer—the curvature seen on log-log plots such as Fig. 12 is a clear indication that data with $1-T/T_c \gtrsim 0.05$ are not within the asymptotic region where the power laws quoted above are valid, and the same problem occurs in Fig. 11. However, with the present simulation techniques the necessary effort in computing time would be prohibitively large: Remember than an increase in program efficiency by about two orders of magnitude was necessary to be able to add about half a decade close to T_c in Figs. 11 and 12 in comparison to previous work[8] with standard programs on scalar computers. Similarly, just half a decade in the bulk magnetic field H can be added in the study of critical wetting, see the Appendix. The challenge put forward by Brézin and Halpin-Healey[14] that one should investigate the region several orders of magnitude closer to the wetting transition certainly cannot be met by the present simulation techniques. In order to make further progress, simulation methods need be developed which eliminate (or strongly reduce) both critical slowing down in the bulk[35] and the slowing down of the interface fluctuations near the free surfaces.

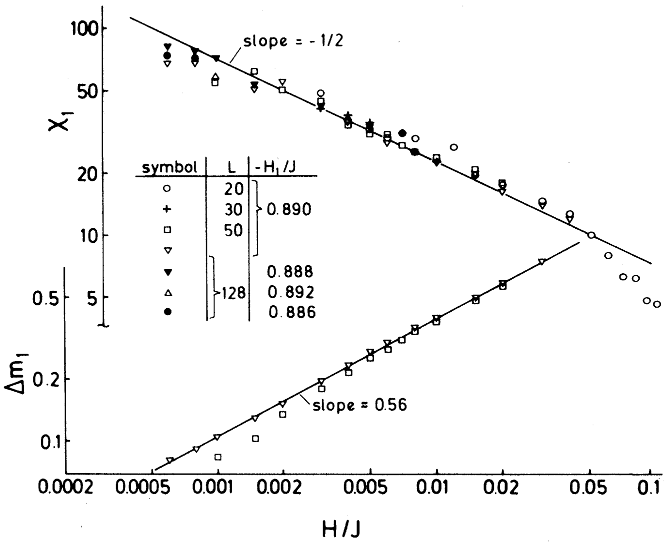

FIG. 14. Surface-layer susceptibility χ_1 (upper part) and excess magnetization Δm_1 (lower part) on a log-log plot vs bulk field at $H_1=H_{1c}$, $J_s=J$, $J/k_BT=0.35$.

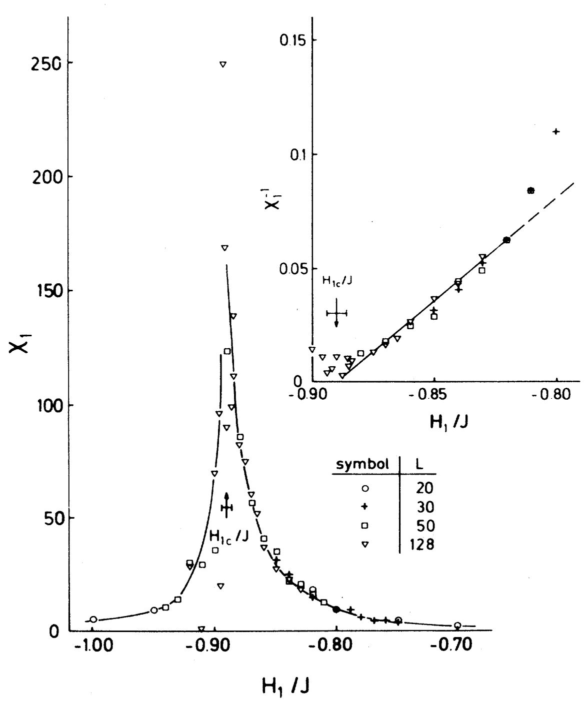

FIG. 13. Surface-layer susceptibility χ_1 plotted vs surface field H_1 at $J_s=J$, $J/k_BT=0.35$, and $H=0$. Insert shows χ_1^{-1} plotted vs H_1/J on an expanded scale. Several choices of L are indicated ($D=40$), as well as the resulting estimate for H_{1c}/J.

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APPENDIX: RECONSIDERATION OF THE CRITICAL BEHAVIOR AT SECOND-ORDER WETTING TRANSITIONS

In our previous work,[7,8] the theoretically predicted[10–13] deviations from mean-field behavior for critical wetting have not been seen. Before one too hastily concludes that the theory is incorrect for the model under consideration, however, one must also consider limitations of the simulations as a possible source of the discrepancy. References 7 and 8 attempted to study the surface-layer susceptibility χ_1 at $H_1=H_{1c}$ as a function of the bulk field, as well as the excess of the surface-layer magnetization $\Delta m_1=m_1(H)-m_1(H=0)$. Apart from possible logarithmic correction factors,[14–17] these quantities should vary as[7,8]

$$\chi_1\sim H^{1/2\nu_\parallel},\quad \Delta m_1\sim H^{1-1/2\nu_\parallel}\,. \tag{A1}$$

While in mean-field theory $\nu_{\parallel}=1$ renormalization-group theory predicts a value of $\nu_{\parallel}$ much larger than unity ($\nu_{\parallel}$ is probably close to 6 for the Ising model).[7,8,17]

Now a Monte Carlo study attempting to verify Eq. (A1) may fail due to the following limitations.

(i) The critical field H_{1c} is not known exactly, but rather it is extracted from the simulations only with appreciable error (see Sec. III). As a consequence, if the simulation is carried out at a value H_1 which is somewhat off the true H_{1c}, misleading results on the variation with H due to crossover effects could be obtained.

(ii) If the analysis is based on a range of field values H which are not small enough, the asymptotic critical region is not reached. In principle, such a problem should show up as a slight curvature on the log-log plots,[14,16] but if the data are too noisy this curvature is easily overlooked. In fact, the data of References 7 and 8 are hampered by rather large statistical errors—neither (i) nor (ii) are ruled out.

(iii) In view of the predicted large values of the correlation length $\xi_{\parallel}$ parallel to the surface, finite-size effects may be a serious problem.

Thus, in order to check for the limitations (i)–(iii), simulations on much larger lattices and with much better statistics than presented in Refs. 7 and 8 are required. We have carried out such simulations for a parameter combination studies previously, $J_s=J$ and $J/k_BT=0.35$: Fig. 13 shows that the new data confirm the previous location of H_{1c}, namely, $H_{1c}/J=-0.89$. With the present data, we feel that a very satisfactory accuracy can be obtained, namely, $\Delta H_{1c}/J\approx\pm0.004$, i.e., less than half a percent relative error. Thus, problem (i) is unlikely to be the main problem. Figure 14 shows that problems (ii) and (iii) do not seem to be the source of the discrepancy either: The more accurate data for $L=128$ do confirm the previous estimates that $\nu_{\parallel}=1$ (or at least very close to this mean-field value). In the accessible part of the "critical regime," i.e., $0.0006\le H/J\le 0.05$, we see a rather good straight-line behavior over nearly two decades. However, it clearly is not possible to approach the wetting transition even closer: For fields $H/J<0.0010$ the data for χ_1 start to depend on the precise choice of H_1 within the acceptable error ΔH_{1c}, as quoted above. Thus, we can exclude a value of $\nu_{\parallel}$ significantly larger than unity for $H/J\gtrsim 0.001$ only—it is possible that for $H/J<0.001$ a crossover to a larger value of $\nu_{\parallel}$ sets in. We do not think, however, that our data can give any evidence on this problem—for $H/J=0.0006$ we may also start to see some finite-size effects.

At this point, we also comment on a question that is sometimes raised, namely, whether the fluctuations are affected by the fact that metastable states are simulated for very small fields ($H\le H_c$, see Ref. 8) rather than truly stable ones: First of all, there is no reason that this should lead to mean-field behavior; secondly, since $H_c\sim 1/D$, one then should see some differences between simulations with $D=40$ and simulations with $D=80$, but no such differences are seen.

In summary, the reanalysis of our previous study[7,8] with much larger lattices ($L=128$ instead of $L=50$) and much better statistics confirm, that for fields $H/J\gtrsim 0.001$ there are about one and a half decades where the critical behavior is described by the mean-field exponents $\nu_{\parallel}=1$. Of course, we cannot tell whether anything new and different happens many decades closer to the transition, as suggested in Ref. 14.

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