Nonclassical wetting behavior in the solid-on-solid limit of the three-dimensional Ising model

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Critical and complete wetting transitions are studied in the solid-on-solid limit of the three-dimensional Ising model. The surface order parameter and coverage are calculated using Monte Carlo methods for various $T > T_R$ (the roughening temperature). The critical behavior is found to be universal but consistent with renormalization-group predictions. We predict that for $T \gtrsim T_R$: (i) the parameter $\omega \simeq \frac{1}{4}$ in the Ising model; this is much less than the previous estimate $\omega \simeq 1$; (ii) the length scale in the effective interface potential is about twice as large as the Ising bulk correlation length.

Wetting phenomena occur when the contact region separating two distinct bulk phases α and γ contains a layer or film of a third phase β. Often, one of the two bulk phases, say γ, is an inert spectator phase which does not equilibrate with the α and β phases on experimentally relevant time scales. This is the case, for example, for multilayer adsorption on an inert solid substrate and for the surface melting of a low-vapor-pressure solid in contact with an inert vapor phase or vacuum.

From the theoretical point of view, the simplest realization of such systems is the semi-infinite Ising model with nearest-neighbor interactions. In this model, the influence of the spectator phase is modeled by an effective surface field which favors the formation of a β layer of, say, down spins between the surface and the bulk up-spin α phase. For spatial dimension $d=2$, this model can be solved exactly, and is known to lead to a line of critical wetting transitions characterized by universal exponents.[1] For short-range forces, similar universal wetting behavior is, in fact, expected for all dimensions $1<d<3$.[2] However, for the physically most relevant case $d=3$, the wetting behavior is still a matter of controversy. While renormalization group (RG) (Refs. 3–5) and Monte Carlo (MC) (Ref. 6) studies of Gaussian interface models indicate rather unusual nonuniversal critical behavior, the results of recent Monte Carlo simulations of wetting in the 3D Ising model[7] are consistent with the (universal) predictions of mean-field (MF) theory.

A possible explanation of this discrepancy is that the asymptotic scaling region is very small in the 3D Ising model and has not been reached in the simulations of Ref. 7. Indeed, a Ginzburg criterion has been used[8] to estimate that the crossover from MF to nonclassical behavior was not yet reached in the simulations of Binder and coworkers.[7] A somewhat contradictory result has been obtained from a numerical solution of the functional renormalization-group equations:[6,9] A broad crossover region is predicted, with measurable deviations from MF behavior even at rather large values of the reduced fields. Neither approach is, however, conclusive because the predictions depend on the values of various unknown model-dependent parameters. Furthermore, both results are based on analyses of the Gaussian interface model, which may not, in fact, capture the physics of wetting in the 3D Ising model.

In order to resolve this discrepancy, we consider here the solid-on-solid (SOS) limit of the 3D nearest-neighbor Ising model on a cubic lattice with a (100) surface. On the one hand, this model is close enough to the original Ising model to allow a direct comparison of nonuniversal quantities. On the other hand, it is simple enough that much larger lattices (and smaller fields) can be simulated. Restricting ourselves to the case in which the coupling constant at the surface (J_s) equals that in the bulk (J), our Hamiltonian is given by

$$\mathcal{H}/T=(2J/T)\sum_{\langle ij\rangle}|z_i-z_j|+\sum_i V(z_i)/T\,, \tag{1}$$

where the discrete variables $z_i=0,1,2,\ldots$, measure the local distance of the (α,β) interface from the surface in units of the lattice parameter a. The second term in (1) represents the direct interaction of the interface with the surface. It has the form

$$V(z)=2Hz+2H_1\delta_{z,0}\,, \tag{2}$$

where H and H_1 are the bulk and surface fields in the original Ising model. In order to investigate the influence of the discreteness of the height variables, we also consider another version of (1) with continuous $z_i \geq 0$ in which the surface field H_1 is mimicked by a square-well potential $W(z)=-W_0$ for $0<z<1$.

As described further below, we have performed extensive MC simulations of this model, both for discrete and continuous z_i. A detailed analysis of our MC data shows that this model belongs to the *same universality class* as the Gaussian interface model described by the effective Hamiltonian

$$\mathcal{H}\{l\}/T=\int d^2x\left[\tfrac{1}{2}(\tilde{\Sigma}/T)(\nabla l)^2+U(l)\right] \tag{3}$$

for the variable $l \equiv az$, with the interfacial stiffness $\tilde{\Sigma}/T = c_1 (J/Ta)^2$ and $c_1 \simeq 10.4$. The direct interaction potential $U(l)$ has the form

$$U(l) \approx hl - Ae^{-l/\xi a} + Be^{-2l/\xi a} \qquad (4)$$

for large l, where $h \simeq 2H/Ta^2$ and the length scale ξ is given by $\xi = c_2 T/J$ with $c_2 \simeq 0.175$.[10] The amplitude A is proportional to the deviation of the surface field from its value at criticality: $A \sim H_{1c}(T) - H_1$. Thus, we find that the dimensionless parameter $\omega \equiv T/4\pi\tilde{\Sigma}a^2\xi^2$ which determines the singular behavior at the wetting transition has the *universal* value $\omega \simeq \frac{1}{4}$ for the Ising model in the SOS limit.

The Gaussian interface model defined by (3) and (4) should be regarded as the coarse-grained version of (1) and (2). In the SOS model, the interface has an intrinsic width which is set by the lattice parameter a. In the process of eliminating short-wavelength interface fluctuations, this width increases to ξ. In the Gaussian interface model previously investigated,[3-5] the scale ξ is replaced by the bulk correlation length ξ_b. The latter scale is determined, in part, by interfacial overhangs and droplet excitations which are ignored in the SOS limit.

The SOS model represents a low-temperature approximation to the Ising model. We are concerned here with critical wetting transitions which occur for $T > T_R$, where $J/T_R \simeq 0.41$ is the Ising model roughening temperature. *A priori* it is not clear if the SOS limit is still a good approximation for such temperatures. However, we estimate that the parameters ξ and Σ/T obtained for the SOS model are in reasonably good agreement with the corresponding quantities for the Ising model, as derived from the wetting simulation data,[7] at temperatures $J/T \simeq 0.35$. This allows us to make two predictions concerning critical wetting behavior in the 3D Ising model: (i) The dimensionless parameter ω is approximately equal to $\frac{1}{4}$ for $J/T \simeq 0.35$, i.e., is much smaller than the previous estimate $\omega \simeq 1$.[7] This implies that the length scale ξ is about *twice* as large as the bulk correlation length of the Ising model[11] at this temperature. (ii) In order to observe deviations from MF critical behavior and enter the asymptotic scaling regime in MC simulations of the 3D Ising model, one needs to study lattices with a lateral dimension of at least $L \sim 100$–200.

Simulations were performed on model (1), (2) at $J/T = 0.35$ and 0.175 using an $(L+1)\times L$ square lattice with helical boundary conditions. In the model with continuous z_i, several temperatures, $J/T = 0.125$, 0.175, 0.25, 0.35, and 0.7, were investigated in order to verify the universality properties discussed above. In this case, square lattices containing L^2 sites with periodic boundary conditions were used. Lattice sizes up to $L = 200$ were employed and generally on the order of 10^6 MC updates per site were used in evaluating the averages. Speeds of over 10^6 updates/sec were obtained on a Cray X-MP using a fully vectorized code.

In *all* cases we find that for $H = 0$, a plot of $e^{-J\langle z\rangle/0.35T}$ vs H_1/J (or W_0/J) is asymptotically a straight line. We determined the critical values of the surface field in this way to be $H_{1c}/J \simeq -0.897$ for $J/T = 0.35$ and $H_{1c}/J \simeq -0.086$ for $J/T = 0.175$. Plots of $\langle z\rangle$ and $\log_{10}(\Delta m_1)$ (where $\Delta m_1 = 1 - \langle \delta_{z,0}\rangle$) vs $\log_{10}(\delta H_1/j)$ are shown in Fig. 1. Asymptotically, we find $\langle z\rangle \approx A_1 \ln(\delta H_1/J) + A_2$ and $\ln(\Delta m_1) \approx M_{\rm cw} \ln(\delta H_1/J)$ with A_1, A_2, and $M_{\rm cw}$ given in Table I. Since $\Delta m_1 \sim (\delta H_1/J)^{\beta_1}$, we thus obtain $\beta_1 \simeq 1.62$ (1.57) for $J/T = 0.35$ (0.175). The difference between these two values for β_1 is not statistically significant. This result for β_1 agrees with the RG theory developed in Refs. 3-5 for a unique value of ω. In particular, for $\omega < \frac{1}{2}$, this theory implies $\beta_1 = (1+\omega)/(1-\omega)$ and $\langle z\rangle/\xi \approx -[(1+2\omega)/(1-\omega)]\ln(\delta H_1/J)$, where ξ is a model-dependent length scale. Thus, we obtain $\omega \simeq 0.24$ (0.22) and $\xi J/T \simeq 0.18$ (0.19) at these two temperatures.

Next, consider field-driven critical wetting, i.e., the singular behavior for $H/J \to 0$ at $H_1 = H_{1c}$. Our results for $\langle z\rangle$ and Δm_1 at $J/T = 0.35$ in this case are shown in Fig. 2. Fits to the asymptotic behavior $\langle z\rangle \approx B_1 \ln(H/J) + B_2$ and $\ln(\Delta m_1) \approx M_{\rm fd} \ln(H/J)$ yield the coefficient listed in Table I. Since we expect $\Delta m_1 \sim (H/J)^{1-1/2\nu_\parallel}$, with $\nu_\parallel = (1-\omega)^{-1}$ and $\langle z\rangle/\xi \approx -\frac{1}{2}(1+2\omega)\ln(H/J)$ for $\omega < \frac{1}{2}$, we obtain $\omega \simeq 0.26$ and $\xi J/T \simeq 0.18$, which is again consistent with our previous results.

As a final check, we have plotted data for $\langle z\rangle$ vs $\log_{10}(H/J)$ obtained at the *complete wetting* transition (using $W_0 = 0$ with continuous z_i) for $J/T = 0.125$ in Fig.

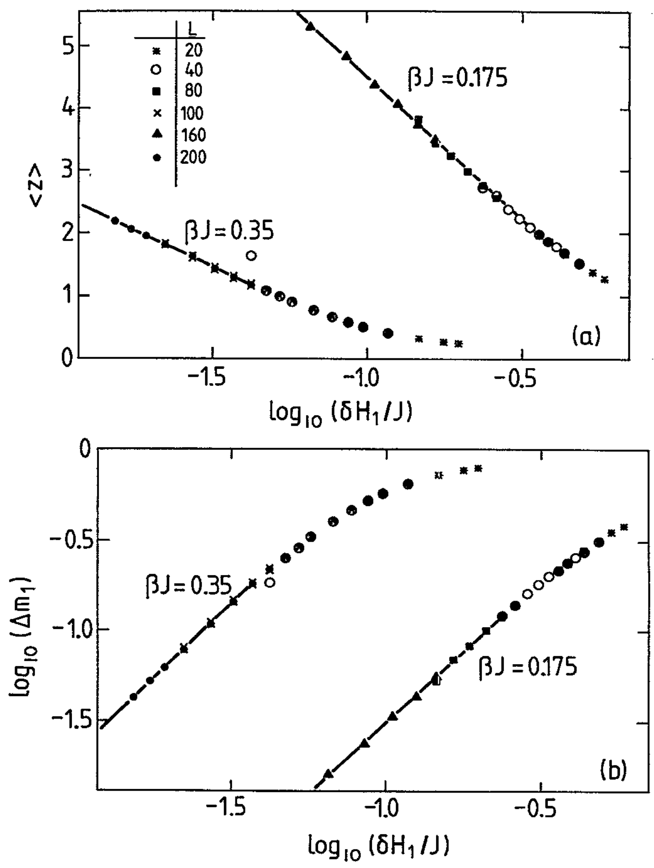

FIG. 1. (a) Coverage $\langle z\rangle$ and (b) logarithm of excess surface order parameter $\log_{10}(\Delta m_1)$ for model (1) at $J/T \equiv \beta J = 0.35$ and 0.175 (and $H = 0$) plotted vs $\log_{10}(\delta H_1/J)$. The solid lines are fits to the asymptotic data described in the text.

TABLE I. Coefficients of fits to the asymptotic behavior of the coverage and $\ln(\Delta m_1)$ at the critical wetting (A_1,A_2,M_{cw}), field-driven critical wetting (B_1,B_2,M_{fd}), and complete wetting (C_1,C_2) transitions.

J/T	A_1	A_2	B_1	B_2	C_1	C_2	M_{cw}	M_{fd}
0.35	−1.00	−2.00	−0.38	−0.48			1.63	0.63
0.175	−1.98	−0.70					1.57	
0.125					−1.57	1.76		

3. A fit to the asymptotic data yields $\langle z\rangle \approx C_1 \ln(H/J) + C_2$, with C_1 and C_2 given in Table I. On the other hand, the above-mentioned RG theory predicts $\langle z\rangle/\xi \approx -\frac{1}{2}(2+\omega)\ln(H/J)$ at the complete wetting transition, so that we obtain $\omega \simeq 0.25$ and $\xi J/T \simeq 0.17$.

All of our results are therefore consistent with the RG predictions for $\omega \simeq \frac{1}{4}$. Several comments are in order. First, note that rather large system sizes are required to determine the critical value of the surface field H_{1c}/J. In addition to the fact that $\nu_{\parallel}$ is rather large ($\simeq 1.3$ in the present case), another complicating factor is that for $H=0$, static expectation values of many quantities are well defined only in the thermodynamic limit. In fact, for $H=0$ and any finite $L \gg \xi_{\parallel}$, there is an exponentially small probability that the interface will "tunnel" out into the wet state.[12] This will almost never happen on normal simulation time scales until $\xi_{\parallel} \lesssim L$. As can be seen from Fig. 1, the requirement $\xi_{\parallel} \lesssim L$ is rather severe. Except for one data point for $L=40$ at $J/T=0.35$, only data unaffected by finite-size effects have been plotted in this figure. For a given lattice size, data taken at smaller values of $\delta H_1/J$ exhibit noticeable deviations from the infinite system behavior. For $L=40$ this means that reliable data can be obtained at $J/T=0.35$ only for $\delta H_1/J \gtrsim 4.5\times 10^{-2}$, and for $L=100$, $\delta H_1/J \gtrsim 2.2\times 10^{-2}$. The asymptotic scaling regime can thus only be entered when L is greater than 40 or 50. This leads us to the conclusion that in the temperature direction (i.e., for $\delta H_1/J \to 0$ at $H=0$), Binder and co-workers[7] have just started to enter the asymptotic regime for their largest system size (for $J/T=0.35$). Nevertheless, their value for the critical surface field, $H_{1c}/J=-0.89$, at this temperature is remarkably close to our value.

In the H direction, $\xi_{\parallel} \sim (H/J)^{-1/2}$ so that the system size requirements are less stringent.[6] Furthermore, one has better control over the finite-size behavior,[12] and it appears that for $J/T=0.35$, Binder and co-workers do indeed enter the asymptotic scaling region in this case.

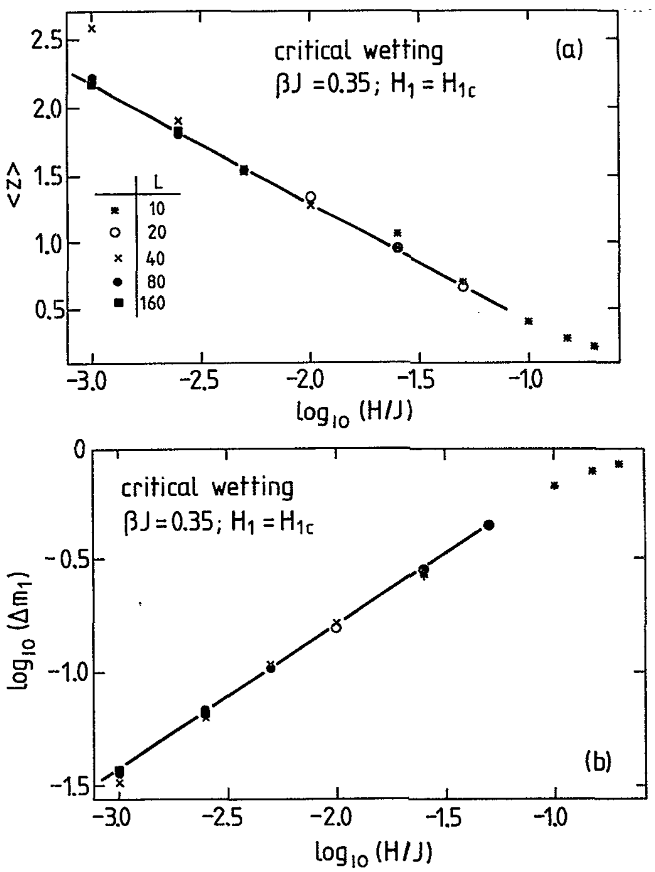

FIG. 2. (a) Coverage $\langle z\rangle$ and (b) logarithm of excess surface parameter $\log_{10}(\Delta m_1)$ for model (1) at $J/T \equiv \beta J = 0.35$ (and $H_1 = H_{1c}$) plotted vs $\log_{10}(H/J)$. The solid lines are fits to the asymptotic data as described in the text. The deviations of the data from the fit at small H/J are due to finite-size effects (see Ref. 11).

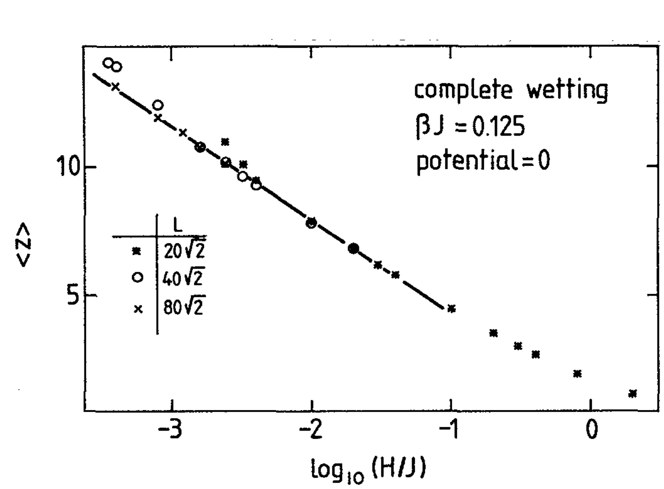

FIG. 3. Coverage $\langle z\rangle$ for $J/T \equiv \beta J = 0.125$ at the complete wetting transition ($W_0 \equiv 0$ and continuous z_i) plotted vs $\log_{10}(H/J)$. The solid line is a fit to the asymptotic data. The deviations of the data from the fit curve at small H/J are due to finite-size effects (see Ref. 11).

The coverage m_s which they measure is related to the mean distance $\langle z \rangle$ of the interface from the surface by $m_s \approx 2M \langle z \rangle$, where M is the bulk magnetization. The data for m_s in Fig. 1(a) of Ref. 7(a) (field driven critical wetting) thus yields $\langle z \rangle \approx -0.35 \ln(H/J)$. Assuming $\omega \simeq \frac{1}{4}$, this implies that the length scale ξ discussed above is approximately equal to 0.46 in this case, in surprisingly good agreement with the value 0.5 we obtain from our data. Identifying this length scale with the bulk correlation length $\xi_b \simeq 0.3$, however, does not allow for a consistent interpretation of the data. It should also be mentioned that the finite-size effects they observe for $H/J \to 0$ at $H_1 = H_{1c}$ are in agreement with what we find [compare Fig. 1(a) of Ref. 7(a) with our Fig. 2], indicating that $\xi_{\parallel}$ is approximately the same in both cases. Finally, note that the data for Δm_1 (at $J/T = 0.35$) in Fig. 9(c) of Ref. 7(b) is also consistent with $\omega \simeq \frac{1}{4}$. This makes us reasonably confident that $\omega \simeq 0.25$ at $J/T = 0.35$ in the 3D nearest-neighbor Ising model.[13] However, as discussed above, lattices with a lateral dimension L on the order of 100–200 will probably be required to confirm this behavior.

It would be extremely interesting to have a quantitative RG or coarse-graining procedure to map the SOS Hamiltonian onto model (3), (4). A simple Migdal-Kadanoff procedure does indeed generate a single-site potential similar to (4) as the SOS interaction term is mapped into the Gaussian fixed-point potential; however, the resulting recursion relations are only qualitatively correct and do not indicate why $\omega \simeq \frac{1}{4}$ in this case.

In summary, we have shown that the SOS model for wetting in $d = 3$ belongs to the same universality class as the effective interface model (3) with $\omega \simeq \frac{1}{4}$ for all temperatures $T > T_R$. On the other hand, a detailed comparison of our data with the MC data of Ref. 7 indicates that the SOS model is a good approximation to the Ising model for $T \gtrsim T_R$. This implies that near the roughening temperature the length scale ξ in the interface potential (4) is about twice as large as the bulk correlation length. In contrast to previous estimates we therefore conclude that the parameter ω is indeed $\omega \simeq \frac{1}{4}$ for $T \gtrsim T_R$.

An open question which still needs to be resolved concerns the value of $\omega(T)$ for the 3D nearest-neighbor Ising model in the temperature regime $J/T_c < J/T < 0.35$. Although ω is believed to be of order 1 at T_c, the data in Ref. 7 give no indication that ω is larger for $J/T = 0.25$ than for 0.35. Our work indicates that it should be possible to resolve this question in the near future using highly optimized vectorized codes on a supercomputer.

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[10]This "universality" can be understood by considering the effect of absorbing the coupling constant J/T in the height variables z_i. In the continuum version (i.e., when $\{z_i\}$ are continuous variables), this results simply in a rescaling of the width of the square-well potential $W(z)$. While this may change the width of the scaling region, it should not effect the asymptotic critical behavior. Thus, *if the discreteness of the height variables z_i is irrelevant,* the critical wetting behavior associated with (1) and (2) is the same for all temperatures. We have found that this is indeed the case for all $J/T \geq 0.35$ (the lowest temperature studied). It is somewhat surprising that the effect of the discreteness of $\{z_i\}$ is negligible so close to the roughening temperature T_R.

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[13]Our data indicate that the interfacial stiffness $a^2\tilde{\Sigma}/T \simeq 1.27$ at $J/T = 0.35$ [see discussion following Eq. (3)]. The present analysis suggests that this is a reliable estimate for the stiffness in the 3D Ising model at this temperature. Note that this is only about 20% less than its universal value $a^2\tilde{\Sigma}/T_R = \pi/2$ at T_R^+.