Monte Carlo studies of anisotropic surface tension and interfacial roughening in the three-dimensional Ising model

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Extensive Monte Carlo simulations of the simple cubic Ising model with nearest-neighbor ferromagnetic interactions with a tilted interface are presented for a wide range of lattice size L, temperature T, and tilt angles θ . The anisotropic interfacial tension is studied in detail. From the small-angle data, we obtain the step free energy density $f_S(T,L)$. Finite-size scaling of the step free energy density is discussed and used to probe the predicted temperature dependence of the correlation length near and above the roughening transition. The square-root temperature dependence predicted by solid-on-solid model calculations is exhibited. Finite-size scaling implies that the step free energy varies as 1/L in the rough phase, and thus the applicability of a capillary wave Hamiltonian to describe interfaces of lattice models needs careful discussion.

I. INTRODUCTION

The coexistence of domains of different phases in systems that can undergo phase transitions is a frequent phenomenon and relevant for many properties of these systems. The study of surfaces and interfaces thus constitutes a topic of considerable interest.¹ The nature of the coexistence is governed by the excess thermodynamic properties due to the presence of the interface. The normalized excess free energy per unit area of the interface is defined to be the surface tension and is important in understanding interfacial phenomena. For many physical systems with discrete symmetry, such as lattice models and crystalline solids, the orientation of the interfaces or the anisotropy of the interfacial tension can play a substantial role for many phenomena, including equilibrium crystal shapes, free energy barriers for the nucleation of a crystallite from another crystalline phase, and the interfacial roughening transition.²

For bulk dimensions larger than two, the interface separating ordered domains undergoes a finite temperature roughening phase transition, from a smooth to a rough interface. The interface is rough in the sense that the root-mean-squared width of the interface diverges for a system in the thermodynamic limit at and above the roughening transition. Below the roughening temperature the interface is completely flat, apart from welllocalized small scale excursions. The linear dimension of these interface excitations in directions parallel to the interface is typically of the size of a correlation length, which diverges at the roughening temperature T_R . At and above T_R , excitations of infinite size (steps running across the interface) occur. The unbounded proliferation of such excitations is possible only for vanishing excess step free energy. This mechanism is responsible for the disappearance of facets in the crystal faceting transition.

Since a flat interface with a single step represents an interface with a small tilt, the connection of the step free energy to the linear term in a Taylor expansion of the anisotropic surface tensions in powers of the tilt angle becomes evident. Above the roughening transition, multiple steps form at the interface and control the interfacial excitations. This is often modeled by the capillary wave spectrum of an interface with continuous symmetry. Such modeling plays an important role in numerous applications, such as in the description of wetting phenomena.³ There, one of two phases preferentially wets a substrate or a third phase. Wetting phenomena have been the subject of extensive theoretical and experimental research.

In a recent letter, ⁴ we have presented the main results of an extensive Monte Carlo study of the anisotropic interfacial tension for the simple cubic Ising model using a wide range of lattice sizes, temperatures, and tilt angles. The finite-size dependence of the step free energy has been obtained and used to probe the temperature dependence of the correlation length near the roughening transition. Implications on the applicability of the capillary wave Hamiltonian approximation to wetting phenomena in lattice models have also been considered. In fact, the recent failure⁵ to verify renormalization group predictions on critical wetting⁶ in an Ising model simulation was a major motivation for this work, since lattice effects might be responsible for this discrepancy. This problem is still a subject of current research.⁷⁻⁹

The present paper now gives a more detailed description of the work briefly mentioned in Ref. 4. In the next section, we briefly review the basic theoretical concepts and define our notation. There we first discuss the anisotropic interfacial tension, and its relation to the step free energy and the roughening transition. The predictions for the critical behavior at the roughening transition obtained from solid-on-solid (SOS) model calculations are briefly reviewed, and the concept of finite-size scaling at the roughening transition is outlined. In Sec. III, our Monte Carlo methods are described, while our results are then presented and analyzed in Sec. IV. The paper then concludes in Sec. V with a discussion of our results and with some remarks on the implications on the use of the capillary wave Hamiltonian approximation for lattice models.

II. BASIC THEORETICAL CONCEPTS

A. Anisotropic interfacial free energy

In general, the interfacial excess free energy $F_{\rm ex}$ is defined to be the free energy difference between two systems with and without an interface, produced under appropriate sets of boundary conditions. The interfacial tension τ , then, is obtained by normalization of $F_{\rm ex}$ with the appropriate cross-sectional area.

In systems without full rotational symmetry, we need to introduce an anisotropic interfacial tension to describe interfaces at some orientation relative to a given symmetry direction. For three-dimensional systems, two angles (θ, ϕ) are needed to fully describe an arbitrary orientation of the interface. In the present first calculation of anisotropic interfacial free energies, we restrict ourselves to consider a single angular variable θ only, and set ϕ equal to zero. Thus, θ is the angle by which the interface (which for $\theta=0$ is in the xy plane) is rotated around the x axis of the considered cubic lattice, where x,y,z are the lattice axes. We thus consider the anisotropic interfacial tension

$$\tau(\theta,T) \equiv \tau(\theta,\phi=0,T)$$
,

for the simple cubic nearest-neighbor ferromagnetic Ising model at temperatures T below the bulk critical temperature T_c with an interface separating a domain with positive magnetization (predominantly up spins), from a domain with negative magnetization (predominantly down spins).

The anisotropic interfacial tension $\tau(\theta, \phi, T)$ plays a key role in the theory of the equilibrium shape of crystals, ¹⁰ via the well-known Wulff construction. ¹¹ Here one is particularly interested in the disappearance of crystal facets at the faceting transitions. Suppose we fix the angle ϕ to orient the crystal surface relative to a given axis. The disappearance of a facet of that particular orientation will correspond to the vanishing of a cusp in the polar plot of $\tau(\theta, \phi, T)$. For the surface parallel to the z axis in the simple cubic lattice, this occurs for $\partial \tau(\theta, T)/\partial \theta|_{\theta=0} \rightarrow 0$.

B. Step free energy and roughening transition

At T=0 and $\theta=0$, the interface is perfectly flat. At nonzero but very low temperature, small localized thermal excitations appear at the interface, just as analogous thermal excitations (clusters of overturned spins) appear in the bulk. However, while the bulk excitations grow to macroscopic size (controlled by the bulk correlation length) only at the bulk critical temperature, the interfacial excitations exhibit critical behavior already at the temperature T_R of the roughening transition.

The roughening transition can be characterized by the vanishing of the step free energy per unit length $f_s(T)$, just as the bulk transition can be characterized by the vanishing of the interfacial tension τ . The step free energy for a $L \times L$ interface is the free energy difference of a system with a flat interface and one which has a single step. This latter system, of course, can also be considered as a tilted interface with a tilt angle $\theta = \arctan(1/L)$. Note that throughout this paper lengths are measured in units of the lattice spacing. In the thermodynamic limit, where $L \to \infty$, $f_s(T)$ hence can also be defined as

$$f_s(T) = \frac{\partial \tau(\theta, T)}{\partial \theta} \bigg|_{\theta=0} .$$
⁽¹⁾

In general, a step along arbitrary direction should be considered, however, this is beyond the scope of the present work. While for $T < T_R$ the probability to create a step of length L at a flat interface decreases proportional to

$$\exp[-Lf_s(T)/k_BT]$$
,

the freely occurring step excitations at T_R are responsible for the divergence of the interfacial width at the roughening transition. As mentioned previously, this also leads to a faceting transition in the Ising model.

In spite of their importance, only the ground-state values of $f_s(T=0)=2J$ and

$$\tau(\theta, T=0)=2J(\sin\theta+\cos\theta)$$

are known for the Ising model in the physically most interesting three-dimensional case, while neither $f_s(T)$ nor $\tau(\theta, T)$ are know explicitly at nonzero temperatures. Here J is the exchange constant of the Ising Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} S_i S_j, \quad S_i = \pm 1 , \qquad (2)$$

where the sum extends once over all pairs of nearest neighbors. However, knowledge on the nature of the roughening transition has been established through analytical and numerical studies of the various SOS models of interfaces (without overhangs and bubbles).² Exact solution for the body centered solid-on-solid (BCSOS) model¹² and duality transformation of the discrete Gaussian SOS model¹³ predict that the roughening transition is of the Kosterlitz-Thouless¹⁴ type, i.e., an infinite order transition with an infinite correlation length throughout the rough phase. Numerical evidence from Monte Carlo simulations studying the divergence of the interface¹⁵ and other numerical results for the Ising model is consistent with predictions based on the SOS model and invoking the universality principle. $^{16-18}$ In the SOS models, the correlation length $\xi(T)$ of the height-height correlation function has an exponential divergence^{14, 15}

$$\xi(t) \approx B \exp(At^{-1/2}), \quad T \to 0 , \qquad (3)$$

where A, B are constants and t is a reduced temperature variable, $t = 1 - T/T_R$. The step free energy $f_s(t)$ is now

related to $\xi(t)$ by a sort of hyperscaling relation^{2,19} (C is another constant factor)

$$f_s(t) \approx C[\xi(t)]^{-1}, \quad t > 0$$
, (4)

while for t < 0 we have

$$\xi(t<0) = \infty, \ f_s(t<0) = 0$$
 (5)

By assuming these relations to hold also for Ising model interfaces, we can study the temperature dependence of $\xi(t)$ for $t \rightarrow 0$ by calculating $f_s(t)$ only. In this manner, we do not have to consider the difficult problem to locate the Ising interface in the system and calculate the analog of the height-height correlation function.

C. Finite-size scaling

Since Monte Carlo simulations deal with systems of finite size, the divergence of $\xi(t)$ described by Eq. (3) cannot be directly observed; all critical singularities are rounded off by finite size. A straightforward extension of finite-size scaling theory²⁰ to the present problem yields the prediction for the scaling limit of the singular part of the step free energy

$$f_s^{\text{sing}}(L,t) = C\xi^{-1}(t)X(L/\xi(t)) .$$
(6)

C is a constant which sets the scale for $\xi(t)$ and will be set to unity. Here the scaling function $X(\zeta)$ must have the limits

$$X(\zeta \to \infty) = 1 , \qquad (7a)$$

$$X(\zeta \to 0) \propto \zeta^{-1} . \tag{7b}$$

Equation (7a) is needed to recover Eq. (4) in the thermodynamic limit, Eq. (7b) in order that the singular factor $\xi^{-1}(t)$ in Eq. (6) is cancelled for finite L. This indicates that

$$f_s^{\rm sing}(L,t\leq 0) \propto L^{-1} , \qquad (8)$$

i.e., the step free energy is nonzero and vanishes only as L^{-1} at and above T_R . As noted earlier, this implies that $\tau' = \partial \tau / \partial \partial |_{\theta=0}$ does not vanish either and also scales as L^{-1} . Of course, for a finite system only discrete tilt angles $\theta_n = \tan^{-1}(n/L)$ exist, and rather than differentials we have to work with finite differences,

$$\tau^{(n)} = [\tau(\theta_n) - \tau(\theta_{n-1})] / (\theta_n - \theta_{n-1}), \quad n = 1, 2, \dots,$$
(9)

we thus have to assume that $d\tau(\theta)/d\theta$ can be defined sensibly in terms of $\tau^{(n)}$ as given by Eq. (9) with the help of analytic continuation.

Now, Eq. (8) is in principle incomplete since it disregards various logarithmic corrections.²¹ Equation (8) is not even the leading term of the total finite-size contribution to $f_s(L,t)$, which has terms like

$$f_s(L,t \le 0) = k_B T \ln L / L \quad (10)$$

Equation (10) is due to the translational degree of freedom of the step, which can be at any position $1, 2, \ldots, L$, and hence an entropy $\ln L$ is involved. Other finite-size logarithmic corrections are due to capillary waves and in two-dimensional systems can be rigorously established.²² However, all such terms are linear in temperature and are not included in our method of thermodynamic integration.

III. MONTE CARLO METHOD

We considered $L \times L \times L$ simple cubic lattices under two sets of boundary conditions to simulate systems with and without a tilted interface, for temperature $(T^* = T/T_c)$ below the Ising transition of

$$J/k_B T_c = 0.221655$$

(Ref. 23). We chose a rather unusual combination of boundary conditions for this study because of the specific situation which we wanted to model. For the lattices with the tilted interface we imposed an antiperiodic boundary condition (APBC) in the z direction, and this has the effect of producing an interface. The interface is not pinned to a particular equilibrium position but it can wander and is translationally invariant. Thus it is difficult to define and measure the interfacial width unambiguously, but we have not artificially suppressed any fluctuations. An ordinary periodic boundary condition (PBC) is used in the y direction and the interface is tilted by applying a screw periodic boundary condition (SPBC) in the x direction. As a result, we could produce a tilted interface with the tilt angle of $\theta = \tan^{-1}(N_{\theta}/L)$, between 0° and 90° is obtained. N_{θ} is the shift in units of lattice constants in the screw boundary condition (see Fig. 1). The energy difference between this system and an identical system but replacing the antiperiodic by a periodic boundary condition, yields the excess interfacial energy

$$\Delta U_{\text{ex}}(\theta, T^*, L) = U_{\text{APBC}}(\theta, T^*, L) - U_{\text{PBC}}(\theta, T^*, L) . \quad (11)$$

(Note that the system with no interface now has two simple periodic boundary conditions and one screw periodic



FIG. 1. Boundary condition used to impose a tilted interface: Antiperiodic in the z direction, periodic in the y direction, and screw periodic boundary condition in the x direction.

Data were obtained using an ultrafast multispin vectorized code implemented on the Cyber 205 which had a speed up to 30×10^6 updates/second.²⁵ System sizes between L = 16 and L = 96 were used so that finite lattice size behavior could be carefully analyzed. Typically, runs of 10^5 Monte Carlo steps (MCS) per data point were used, with as many as the first 30 000 MCS discarded before data were kept for computing equilibrium properties. Block averages, over 8000 MCS were computed and checked for systematic variations and two or three additional runs were made for a number of points to check for long-time scale relaxation effects and provide an additional estimate of the statistical accuracy. We saw no indication of any residual relaxation, however, there could conceivably still be undetected effects due to processes with characteristic times substantially greater than 10^5 MCS.

IV. RESULTS

In Fig. 2 we present data for the anisotropic interfacial tension $\tau(\theta, T^*, L=32)$ for a wide range of θ and T^* . τ is measured in units of J. A rapid decrease of the slope near $\theta=0$ with increasing T^* is evident, and as discussed



FIG. 2. Angle dependence of the (anisotropic) interfacial tension in units of J. The reduced temperature $T^* = T/T_c$. The solid curve is the theoretical variation, and the dashed lines are added as a guide to the eye.

herein, indeed scales as L^{-1} near T_R^* . For larger angles, the convergence in sizes is very rapid as indicated by $\theta = 29.3^\circ$, where the estimates for L = 64 are already indistinguishable from L = 32 within the estimated errors of about 2%. As the temperature increases, finite-size effects for the small-angle data, shown in Fig. 3, increase. Notice that at $T^* = 0.54$, which is quite close to T_R^* , the curvature of a smooth curve through the data points even changes sign for sufficiently large L. In Fig. 4, we show $\tau(\theta, T^*, L)$ versus T^* for values of θ and L. Good agreement with previous Monte Carlo calculations of $\theta = 0$ is obtained. Note that τ does not exhibit a noticeable singularity at the roughening transition. This is expected from the essential singularity of the transition.

There are two main sources of errors in these results. The first is statistical sampling and is estimated by standard block averaging. Near and above the transition, critical slowing down associated with the interface fluctuations leads to very long-time correlations between the sequentially generated states. Therefore, we have not attempted to study $\tau(\theta, T^*, L)$ at higher temperature and larger system sizes.

The second source of errors comes from performing thermodynamic integrations using discrete grid spacing



FIG. 3. Variation of the angle dependence of the (anisotropic) interfacial tension for small angles. Solid curves are added as a guide to the eye: (a) $T^* = T/T_c = 0.50$; (b) $T^* = T/T_c = 0.54$. The dashed line is straight.

with only a finite set of data points. Estimates for this were obtained by changing the grid spacing and using a different numerical integration scheme. Both Simpson and Newton integration have been used, with Simpson being the more accurate. All results presented are obtained by Simpson integration. The error of integration is about an order of magnitude larger than sampling errors for the system sizes and Monte Carlo steps considered at temperature near the transition. For example, the error estimated for integration is about 0.05 for L = 96 at $T^* = 0.60$ for the step free energy. The error from sampling is about 0.005. A table of energy for some values of θ and L = 48 is given in Table I for temperatures from $T^* = 0$ to 0.60. These are typical data used in the thermodynamic integration.

We also note that our step free energy does not reflect the degenerate ground-state entropy, which arises from the different possible position of the step. Our boundary



FIG. 4. Surface tension for various angles vs temperatures. The roughening temperature is indicated by an arrow. (a) L = 48, (b) L = 32 and including larger angles.

condition does not pin the step position. This degeneracy would enter as a term linear in temperature, which is nonvanishing for finite system sizes; $k_B T \ln L/L$. Such terms would have been added to the reference free energy density at zero temperature. Since its origin is clear and it would only complicate the finite-size scaling analysis near the roughening transition, we have not included it in our calculation of the step free energy, which should be properly called the *excess* step free energy.

Using our results for $\tau(\theta, L, T^*)$, we obtained the step free energy density $f_s(L,t)$ for L = 16, 32, 48, 64, and 96. This is given in units of J with the lattice space set equal to unity in Fig. 5 as a function of T^* . The estimated error is 0.01 for L = 16 and increases to 0.06 for L = 96 in the regime of interest near the transition. The approaching transition is signaled by the rapid decreases of $f_s(L,t)$ near $T^* \sim 0.5$ and the increases in the finite-size dependence as indicated by the data for different sizes. To apply finite-size scaling [Eq. (3)], we need the temperature dependence of $\xi(t)$ for t < 0. We have extrapolated $f_s(L,t)$ to $L \to \infty$, by assuming a L^{-1} dependence (see Fig. 6). We have no rigorous arguments for the L^{-1} dependence, except that it is correct in the $t \rightarrow 0$ scaling limit. Using the extrapolated values of $f_s(\infty, t)$, we plot the log of $f_s(\infty,t)$ versus $(\sqrt{t})^{-1}$ with different trial values of T_R^* (see Fig. 7). A good linear fit is obtained for $T_R^* = 0.54$, using the data closest to T_R^* . The estimated error for T_R^* is ± 0.02 and is within previous estimates of 0.56 ± 0.03 . The slope of the linear fit gives $A = 1.36 \pm 0.06$ and $B = 9.84 \pm 2.0$ for $\xi(t)$ in Eq. (1).

Given the rather small number of points for each temperature that is in the scaling limit, the extrapolations in Fig. 5 need not be unique. We check that finite-size scaling is obeyed by plotting $[f_s(L,t)\xi(t)]-1$ versus $L/\xi(t)$ in Fig. 8. The data scale satisfactory and are consistent with the L^{-1} dependence assumed in the extrapolation. Thus, an alternative description of data analysis is that we have fitted data with three parameters, T_R^* , A, and Bwith the constraint that Eqs. (1) and (3) be satisfied. It would have been more satisfying to increase the number of data points for larger sizes and reducing the error estimates, but these initial calculations already consumed on the order of 1000 CPU h on the Cyber 205 with an ultrafast multispin vectorized code.

One of the applications of our results is to study the functional dependence of $\tau(\theta, T^*, L)$ on θ near $\theta=0$. This would be relevant for discussions of capillary wave Hamiltonian approximations above the roughening transition. In that context the higher derivatives of $\tau(\theta, T^*, L)$ with respect to θ are important.²⁶ We have analyzed our data by fitting the small θ results to

$$\theta, T^*, L) = \tau(0, T^*, L) + \tau'(0, T^*, L) |\theta| + \tau''(0, T^*, L) \frac{\theta^2}{2} .$$
(12)

 τ (

Ignoring higher-order terms, we find that τ'' is negative for low *T*, but crosses to positive values near T_R^* (see Fig. 9). This behavior is consistent with the mechanical stability requirement of the interface. It is also a very

<i>T</i> *	$0.0^{\circ}, L = 48$		1.19°, $L = 48$		2.38°, $L = 48$	
	$U_{ m APBC}$	$U_{ m PBC}$	U_{APBC}	$U_{ m PBC}$	$U_{ m APBC}$	$U_{ m PBC}$
0.00	-2.958 83	-3.00000	-2.95747	-3.00000	-2.956 60	-3.00000
0.02	-2.95833	-3.00000	-2.95747	-3.00000	-2.95660	-3.00000
0.04	-2.95833	-3.00000	-2.95747	-3.00000	-2.95660	-3.00000
0.06	-2.95833	-3.00000	-2.95747	-3.00000	-2.95660	- 3.000 00
0.08	-2.95833	-3.00000	-2.95747	-3.00000	-2.95660	-3.00000
0.10	-2.95833	-3.00000	-2.95746	-3.00000	-2.956 59	-3.00000
0.12	-2.95833	-3.00000	-2.95744	-3.00000	-2.95655	-3.00000
0.14	-2.95833	-3.00000	-2.95740	-3.00000	-2.95647	-3.00000
0.16	-2.95833	-3.00000	-2.95736	-3.00000	-2.95639	-3.00000
0.18	-2.95831	-2.999 99	-2.95730	-2.999 99	-2.95630	- 2.999 99
0.20	-2.95826	-2.999 98	-2.95722	-2.999 98	-2.95617	-2.999 98
0.22	-2.95815	-2.999 93	-2.95707	-2.99993	-2.95597	-2.999 93
0.24	-2.95793	-2.999 81	-2.95680	-2.99981	-2.95566	-2.999 81
0.26	-2.95750	-2.999 56	-2.95633	-2.999 56	-2.95515	-2.999 56
0.28	-2.95677	-2.999 08	-2.955 54	-2.99908	-2.95433	-2.999 08
0.30	-2.955 61	-2.99828	-2.95434	-2.99828	-2.95308	-2.998 28
0.32	-2.95382	-2.996 99	-2.952 51	-2.996 99	-2.95122	-2.996 99
0.34	-2.95126	-2.99506	-2.949 91	-2.99506	-2.94857	-2.995 06
0.36	-2.94769	-2.99231	-2.94631	-2.992 31	-2.94493	-2.992 31
0.38	-2.942 92	-2.98857	-2.94249	-2.98857	-2.94010	-2.98857
0.40	-2.93666	-2.98361	-2.93523	-2.98361	-2.93381	-2.98361
0.42	-2.92873	-2.97725	-2.92727	-2.97725	-2.92582	-2.97725
0.44	-2.91876	-2.96924	-2.91733	-2.969 24	-2.915 92	-2.96924
0.46	-2.90657	-2.95942	-2.90518	-2.95942	-2.90385	-2.95942
0.48	-2.89182	-2.94755	-2.89056	-2.94755	-2.88930	-2.94755
0.50	-2.87427	-2.93345	-2.87327	-2.93345	-2.87234	-2.93345
0.52	-2.85392	-2.91696	-2.85338	-2.91696	-2.85282	-2.91696
0.54	-2.83138	-2.89785	-2.83118	-2.89785	-2.83083	-2.89785
0.56	-2.80659	-2.87586	-2.80646	-2.87586	-2.80626	-2.87586
0.58	-2.77908	-2.85081	-2.77900	-2.85081	-2.77885	-2.85081
0.60	-2.74858	-2.82255	-2.74861	-2.82255	-2.74845	-2.82255

TABLE I. The energy per spin in units of $J/k_B T_c$ for L = 48 with an interface and without an interface.

difficult quantity to obtain accurately using the present methods. We have, in fact, to extract a second derivative numerically, which is much limited by our numerical errors. For this reason, we have not considered a detailed finite-size scaling analysis at this point.



FIG. 5. Temperature dependence of the step free energy $f_s(L, T)$ in units of J per unit lattice spacing. The roughening temperature is indicated by an arrow.



FIG. 6. Size dependence of the step free energy $f_s(L,T)$ in units of J per unit lattice spacing. The straight solid lines show linear extrapolations.



FIG. 7. Log of step free energy per unit length of steps vs $(\sqrt{t})^{-1}$ for $t=1-T^*/T_R^*$ with different trial values of T_R^* . The solid line is the best linear fit obtained.

V. DISCUSSION

It is clear from our results that there are substantial finite-size effects near and above the roughening transition. This demonstration by our data, with the verification of finite-size scaling and SOS model predictions are the main contributions of our work. One can explore numerous problems for a possible implication. Consider the recent renormalization group application of capillary wave Hamiltonian to describe interfaces of lattice models for critical wetting phenomena.⁶ The anisotropic interfacial tension can be expanded for small tilt angles as given in Eq. 12. Below T_R^* , the linear term does not vanish and dominates. Above the roughening transition, the linear term vanishes in the thermodynamic limit for fixed but small θ , and for the remaining quadratic



FIG. 8. Finite-size scaling plots of step free energy. See the text. The straight, solid line is a linear fit.



FIG. 9. τ'' for L = 48 and 64 vs temperature. See Eq. (12). The roughening temperature is indicated by an arrow.

term (which now dominates) one argues the applicability of the capillary wave Hamiltonian which is essentially a continuous Gaussian SOS model in which the coupling constant σ is related to the coarse grained anisotropic interfacial tension of the Ising interface. A simple expression for σ in two dimensions²⁶ has been given as

$$\sigma = [\tau_{cg}(0, T^*) + \tau_{cg}''(0, T^*)],$$

assuming Eq. (4) holds for $\tau_{cg}(\theta, T)$ and invoking the ther-modynamic limit with $T_R^*=0$, $\tau'_{cg}=0$. $\tau_{cg}(\theta, T)$ is defined by integrating over short wavelength fluctuations up to a length scale which is at least of the order of the bulk correlation length ξ_b . For d = 3, the expression for σ is more complicated as two angles are needed to describe arbitrary interface orientation, but terms in au_{cg}' are still absent. Since we expect that the L dependences of $\tau_{\rm cg}(\theta, T^*)$ and $\tau(\theta, T^*)$ are qualitatively similar, our results indicate $\tau'_{\rm cg}$ scales as L^{-1} and $\tau''_{\rm cg}$ is positive definite (but finite) in the rough phase. For critical wetting, the long-wavelength excitations are important and θ is of the order of L^{-1} . This implies that for any finite L, the linear term cannot be neglected and may be comparable to the quadratic term. (Additional studies of systems with rectangular cross sections would be desirable to explore the more general effects of finite size.^{27,28} The use of a capillary wave Hamiltonian is thus a questionable approximation except near T_c , where $\xi_b \rightarrow \infty$ and τ is isotropic. Of course, it is not clear as to what extent the linear term is relevant in modifying the results of the renormalization group results and is responsible for the inconsistency with the Monte Carlo simulations.⁵ It is our hope that this work will stimulate research to clarify the effects of anisotropy on the applications of capillary wave Hamiltonian.

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