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The Roughening Transition of the Three-Dimensional Ising Interface: A Monte Carlo Study

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We study the roughening transition of an interface in an Ising system on a 3D simple cubic lattice using a finite-size scaling method. The particular method has recently been proposed and successfully tested for various solid-on-solid models. The basic idea is the matching of the renormalization-groupflow of the interface with that of the exactly solvable body-centered cubic solid-on-solid model. We unambiguously confirm the Kosterlitz–Thouless nature of the roughening transition of the Ising interface. Our result for the inverse transition temperature $K_R = 0.40754(5)$ is almost two orders of magnitude more accurate than the estimate of Mon, Landau, and Stauffer.

KEY WORDS: Ising model; roughening transition; Monte Carlo; finite-size scaling; renormalization group.

1. INTRODUCTION

Interfaces play an essential role in many areas of science. In condensed matter physics, the most prominent examples are surfaces of liquids and solids. In 1951 Burton *et al.*[1] pointed out that a phase transition may occur in the equilibrium structure of crystal surfaces. Such a phase transition from a smooth to a rough surface is called a roughening transition. They viewed a growing layer of a crystal as a two-dimensional Ising model. The part of the layer occupied by atoms is represented by spin $+1$, while the vacancies are represented by spin -1. From the exact solution of the two-dimensional Ising model[2] one then infers the existence of a phase transition. However, this picture of a crystal surface is very crude. Obviously in

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a real crystal surface there is more than just one single incomplete layer of atoms.

A better description of a crystal in equilibrium with its vapor is provided by the three-dimensional Ising model, where spin $+1$ represents a site occupied by an atom, while spin -1 represents a vacancy. The boundary conditions are chosen such that an interface between a region with most spins equal to $+1$ and a region with most spins equal to -1 is present. In 1973 Weeks *et al.*[3] performed a low-temperature expansion for the width of an (001) interface in a three-dimensional Ising model on a simple cubic lattice with isotropic couplings. They obtained a roughening temperature $T_R = 0.57 T_c$, where T_c is the temperature of the bulk phase transition, while the approximation of the interface by the two dimensional Ising model yields $T_R = 0.503 T_c$. The best known value for the inverse of the critical temperature of the three-dimensional Ising model on a simple cubic lattice is given by $\beta = 0.2216546(10)$.[4]

A fairly good approximation of the Ising interface is given by the so-called SOS (solid-on-solid) models. Neglecting overhangs of the interface and bubbles in the bulk, the variables of the two dimensional models give the height of the interface measured above some reference plane. A duality transformation exactly relates these models with two-dimensional XY models.[5] In contrast to the two-dimensional Ising model, which undergoes a second-order phase transition, SOS models, like XY models, are expected to undergo a Kosterlitz–Thouless (KT) phase transition (see, e.g., refs. 6).

The important question is whether overhangs of the interface and bubbles in the bulk phases are irrelevant for the critical behavior of the interface in the Ising model, so that the roughening transition is of KT nature as it is the case for SOS models. Monte Carlo simulations of the interface in a three-dimensional Ising model have been performed in order to answer this questions.[7–9]

However, the numerical determination of the transition temperature and the confirmation of the KT nature of the phase transition has turned out to be extremely difficult. The reason for this problem can be found in the KT theory itself. At the roughening transition corrections are present that vanish logarithmically with the length scale. Therefore for all lattice sizes that can be simulated one is quite far from the Gaussian fixed point that is the basis for the formulas used for fits in refs. 7–9. In order to overcome this problem one has to take into account the logarithmic corrections in the analysis of the data.[10]

However one can do even better. The body-centered-cubic solid-on-solid (BCSOS) model that was introduced by van Beijeren in 1977[11] as a solid-on-solid approximation of an interface in an Ising model on a body-centered cubic lattice on a (001) lattice plane is solved exactly. The BCSOS

model is equivalent to one of the exactly solved vertex models.[12–14] The exact formula for the free energy and the correlation length proves that the model has a KT-type phase transition.

In refs. 15 and 16 it was proposed to match the renormalization group (RG) flow of other SOS models and the Ising interface with that of the BCSOS model. The RG flow is monitored by properly chosen block observables on finite lattices. In order to determine the roughening temperature of an SOS model or the Ising interface one has to find the temperature where the values for the block observables for the BCSOS model at the roughening temperature are reproduced.

This method has been successfully applied to the ASOS (absolute-value SOS) model, the discrete Gaussian model, and the dual of the standard XY model in two dimensions.[15] Preliminary results were also obtained for the Ising interface.[16]

In the present paper we improve the result of ref. 16 by drastically increasing the statistics for the Ising model as well as for the BCSOS model. The largest lattice size considered is increased from $64 \times 64 \times 27$ to $256 \times 256 \times 31$ allowing the direct matching of the Ising interface with the BCSOS model compared with the indirect approach via the ASOS model of ref. 16. The high statistical accuracy needed for the matching method could be obtained in a moderate amount of CPU time (about two months on a workstation) due to the use of highly efficient cluster algorithms for the Ising interface[23] as well as for the BCSOS model.[22]

This paper is organized as follows. In Section 2 we define the models to be studied. We summarize exact results for the BCSOS model[12–14] relevant to our study. We briefly discuss the RG flow diagram of the KT phase transition. In Section 3 we describe the matching method. We give particular emphasis to the special problems arising in the case of the Ising interface. In Section 4 we discuss our numerical results. A comparison with previous Monte Carlo studies is presented in section 5. In Section 6 we give our conclusions and an outlook.

2. THE MODELS

We consider an Ising model on a simple cubic lattice with extension L in the x and y directions and with extension D in the z direction. For reasons given by the algorithm we only consider odd values of D. We have chosen the convention that the z coordinate of the lattice points takes the half-integer values $z = -D/2, \ldots, D/2$. The Ising model is defined by the partition function

$$Z = \sum_{s_i = \pm 1} \exp(-K^{\mathrm{I}} H) \tag{1}$$

where the classical Hamiltonian is given by

$$H = -\sum_{\langle ij \rangle} J_{\langle ij \rangle} s_i s_j \tag{2}$$

where the summation is taken over all nearest neighbor pairs $\langle ij \rangle$ on the lattice, and $K^{\mathrm{I}} = 1/k_{\mathrm{B}}T$ is the normalized inverse temperature. In the x and y directions we consider periodic boundary conditions. In order to create an interface we apply anti-periodic boundary conditions in the remaining z direction. Antiperiodic boundary conditions are defined by $J_{\langle ij \rangle} = -1$ for bonds $\langle ij \rangle$ connecting the lowermost and uppermost planes of the lattice, while all other nearest neighbor pairs keep $J_{\langle ij \rangle} = 1$.

The ASOS model is the solid-on-solid approximation of an interface in an Ising system on a simple cubic lattice on a (001) lattice plane. It is defined by the partition function

$$Z = \sum_{h_i} \exp\left(-K^{\mathrm{ASOS}} \sum_{\langle i,j \rangle} |h_i - h_j| \right) \tag{3}$$

where h_i is integer-valued and the summation is taken over the nearest neighbor pairs of a 2D square lattice. At low temperatures the Ising interface and the ASOS model are related by $2K^{\mathrm{I}} = K^{\mathrm{ASOS}}$.

In the case of the BCSOS model the two-dimensional lattice splits into two sublattices like a checkerboard. In the original formulation, on one of the sublattices the spins take integer values, whereas the spins on the other sublattice take half-integer values. We adopt a different convention: spins on "odd" lattice sites take values of the form $2n + \frac{1}{2}$, and spins on "even" sites are of the form $2n - \frac{1}{2}$, n integer. As a consequence, the effective distribution for block spins (= averages over blocks) will be centered around integer values (instead of half-integer values), and the average of the lowest energy configurations takes integer values as in the case for the ASOS models defined above. The partition function of the BCSOS model can be expressed as

$$Z = \sum_{h} \exp\left(-K^{\mathrm{S}} \sum_{[i,k]} |h_i - h_k| \right) \tag{4}$$

where i and k are next to nearest neighbors. Nearest neighbor spins h_i and h_j obey the constraint $|h_i - h_j| = 1$. Van Beijeren[11] has shown that the configurations of the BCSOS model are in one-to-one correspondence to the configurations of the F model, which is a special six-vertex model. The F model can be solved exactly with transfer matrix methods[12-14]. For our choice of the field variable the roughening coupling is given by

$$K_{\mathrm{R}}^{\mathrm{S}} = \tfrac{1}{2} \ln 2$$

The critical behavior of non-local quantities such as the correlation length ξ is known and has the form predicted by KT theory.[14]

The RG flow of SOS models is well described by two parameters β and y.[6] The two-dimensional sine-Gordon model is especially suited to discuss the flow of these parameters with the length scale, since this model contains β and y as bare parameters in its action. On the lattice it is given by the partition function

$$Z^{SG} = \int [d\phi] \exp\left(-\frac{1}{2\beta} \sum_{\langle i,j \rangle} (\phi_i - \phi_j)^2 + y \sum_i \cos(2\pi\phi_i) \right) \tag{5}$$

where the ϕ_i are real numbers.

For the continuum version of the model with a momentum cutoff one can derive the parameter flow under infinitesimal RG transformations.[6] It is given, to second order in perturbation theory, by

$$\dot{x} = -z^2, \qquad \dot{z} = xz \tag{6}$$

where $z = \text{const} \cdot y$ and $x = \pi\beta - 2$. Here, const depends on the particular cutoff scheme used. The derivative is taken with respect to the logarithm of the cutoff scale. For large x, z flows toward $z = 0$. The large-distance behavior of the model is therefore the same as that of the massless Gaussian model. For small x, z increases with increasing length scale. The theory is therefore massive. The critical trajectory separates these two regions in the coupling space. It ends at a Gaussian fixed point characterized by $x = 0$ or $\beta = 2/\pi$. On the critical trajectory the fugacity vanishes as

$$z(t) = \frac{1}{z_0^{-1} + t} \tag{7}$$

where t is the logarithm of the cutoff scale.

3. THE MATCHING METHOD

In order to compare the RG flows of the Ising interface and the BCSOS model we follow closely the method introduced in ref. 15. This method is closely related to the finite-size scaling methods proposed by Nightingale[19] and Binder.[20] No attempt is made to compute the RG flow of the couplings explicitly, but rather the RG flow is monitored by evaluating quantities that are primarily sensitive to the lowest frequency fluctuations on a finite lattice.

In order to separate the low-frequency modes of the field a block-spin transformation[21] is used. Blocked systems of size $l \times l$ are considered. The size B of a block (measured in units of the original lattice spacing) is then given by $B = L/l$, where L is the linear size of the original lattice. For solid-on-solid models the block spins are defined by

$$\phi_{\tilde{j}} = B^{-2} \sum_{j \in \tilde{j}} h_j \tag{8}$$

where $\tilde{j}$ labels square blocks of a linear extension B. One should note that this linear blocking rule has the half-group property that the successive applications of two transformations with a scale factor of B have exactly the same effect as a single transformation with a scale factor of B^2.

Since the position of the interface in the Ising system is not well defined on a microscopic level, we have to look for a substitute of the blocking rule applied to the field of the SOS models. In the following we briefly discuss the solution of the problem proposed and applied to the study of interfaces in the rough phase in ref. 24.

First we have to ensure that the interface is not located at the $z = -D/2$ to $z = D/2$ boundary, in which case the definition of the block spin discussed below would become meaningless. Therefore we locate the interface in the system in a crude fashion, which is done by searching for the z slice with the smallest absolute value of the magnetization. Then we redefine the z coordinate such that the interface is located close to $z = 0$. Now one can go ahead with the measurement of interface properties, ignoring the periodicity of the lattice in the z direction.

The blocks considered have the full lattice extension D in the z direction and an extension B in x and y directions. The interface position is defined inside a block by

$$\phi_{\tilde{i}} = \frac{M_{\tilde{i}}}{2mB^2} \tag{9}$$

where $M_{\tilde{i}}$ is the total magnetization in the block $\tilde{i}$ and m is the bulk magnetization. This definition is motivated by the naive picture that above the interface the magnetization takes uniformly the value $-m$ and below the value m.

One has to discuss to what extent the meaning of the above definition is spoiled by corrections to this simple picture. What are the effects of bulk fluctuations and overhangs of the interface? The fluctuations of the bulk magnetization are given by the magnetic susceptibility χ. The square of the fluctuations of $M_{\tilde{i}}$ induced by the bulk fluctuation is therefore given by

$\sigma^2(M_{\tilde{i}}) = DB^2\chi$ and the resulting fluctuations of $\phi_{\tilde{i}}$ induced by bulk fluctuations is given by

$$\sigma_b^2(\phi_{\tilde{i}}) = \frac{1}{4}\frac{D}{B^2}\frac{\chi}{m^2} \tag{10}$$

As a consequence, the larger the block size in the x and y directions, the better is the position of the interface defined. However, when D is sent to infinity for a fixed B, the position of the interface defined by Eq. (9) becomes meaningless.

In refs. 23 and 15 we proposed a radical solution to overcome the problem of bulk fluctuations completely. Before the position of the interface is determined all bubbles are removed. Technically this is accomplished by performing standard cluster updates at $K = \infty$. Since the absolute value of the bulk magnetization becomes 1 in this process, the definition of the interface position is modified to

$$\bar{\phi}_{\tilde{i}} = \frac{\bar{M}_{\tilde{i}}}{2B^2} \tag{11}$$

Overhangs of the interface are expected on a scale of the bulk correlation length ξ_b. Therefore we have to assume that the position of the interface only has a well-defined meaning if the block size is large compared with the bulk correlation length $B \gg \xi_b$. At the roughening transition this is, however, no severe restrictions since, $\xi_b \approx 0.3$.

Finally, one should ensure that no additional interfaces are created spontaneously. Following ref. 25, we have that the surface tension at $K^I = 0.40$ is $\sigma = 0.6721(1)$. This is certainly a lower bound for the surface tension at the roughening coupling to be found below. Therefore two additional interfaces are suppressed by at least a factor of $D^2 \exp(-0.6721 \times 2L^2)$, which is certainly sufficient already for the smallest lattice size $L = 32$ that we consider.

Now we define suitable observables for the blocked systems discussed above. Motivated by the perturbation theory of the sine-Gordon model, we choose two types of observables, those "sensitive" to the flow of the kinetic term (flow of K), and those sensitive to the fugacity (periodic perturbation of a massless Gaussian model). For the first type of observables we choose

$$A_1 = \langle (\phi_{\tilde{i}} - \phi_{\tilde{j}}) \rangle \tag{12}$$

where $\tilde{i}$ and $\tilde{j}$ are nearest neighbors on the block lattice, and

$$A_2 = \langle (\phi_{\tilde{i}} - \phi_{\tilde{k}})^2 \rangle \tag{13}$$

where $\tilde{i}$ and $\tilde{k}$ are next nearest neighbors. Note that these quantities are only defined for $l > 1$. As a monitor for the fugacity we take the following set of quantities (defined for $l = 1, 2, 4$):

$$\begin{aligned} A_3 &= \langle \cos(2\pi\phi_{\tilde{i}}) \rangle \\ A_4 &= \langle \cos(2 \cdot 2\pi\phi_{\tilde{i}}) \rangle \\ A_5 &= \langle \cos(3 \cdot 2\pi\phi_{\tilde{i}}) \rangle \end{aligned} \tag{14}$$

3.1. Determination of the Roughening Coupling

As discussed in ref. 15, there are two parameters which have to be adjusted in order to match the RG flow of the Ising interface with that of the critical BCSOS model: The coupling K^{I} of the Ising interface and in addition the ratio $b = B^{\mathrm{I}}/B^{\mathrm{S}} = L^{\mathrm{I}}/L^{\mathrm{S}}$ of the lattice sizes (and hence the block sizes) of the Ising model and the BCSOS model. A $b \neq 1$ is needed to compensate for the different starting points of the two models on the critical RG trajectory. In refs. 15 and 16, $b = 3.3(3)$ was obtained.

For the proper values of the roughening coupling $K_{\mathrm{R}}^{\mathrm{I}}$ and the matching constant b observables of the Ising interface and the BCSOS model match like

$$A^{\mathrm{I}}_{i,l}(bB, K^{\mathrm{I}}_{\mathrm{R}}) = A^{\mathrm{S}}_{i,l}(B, K^{\mathrm{S}}_{\mathrm{R}}) + O(B^{-\omega}) \tag{15}$$

where i indicates the observable and l the size of the blocked lattice. The $O(B^{-\omega})$ corrections are due to irrelevant operators. ω is the correction-to-scaling exponent. The perturbation theory of the sine-Gordon model suggests $\omega = 2$.

In order to obtain a numerical estimate for the roughening coupling $K_{\mathrm{R}}^{\mathrm{I}}$ of the Ising model and the matching factor b for a given lattice size L^{S} of the BCSOS model we require that the equation above is exactly fulfilled for two block observables.

In the following we consider the pairs $(A_{1,l}, A_{3,l})$ and $(A_{2,l}, A_{3,l})$ for $l = 2$ and $l = 4$. Replacing $A_{3,l}$ by $A_{4,l}$ or $A_{5,l}$ leads to statistically poorer results.

We solved the system of two equations for the two observables $A_{i,l}$ and $A_{j,l}$ numerically by first computing the $K^{\mathrm{I}}_{i,l}(b)$ and $K^{\mathrm{I}}_{j,l}(b)$ that solve the single equations for a given value of b. The intersection of the two curves $K^{\mathrm{I}}_{i,l}(b)$ and $K^{\mathrm{I}}_{j,l}(b)$ gives us then the solution of the system of two equations. For an illustration of this method see Figs. 5 and 6 of ref. 15.

In ref. 15 it was demonstrated that the corrections to scaling for the observables A_1 and A_2 for SOS models are similar to those in the massless continuous Gaussian model. Therefore we considered the "improved" observable D_1 which is defined as follows:

$$D_1(L) = \frac{A_1^{(0)}(\infty)}{A_1^{(0)}(L)} A_1(L) \tag{16}$$

$A_1^{(0)}$ is computed for the massless Gaussian model defined by

$$Z_0 = \int \prod_x d\psi_x \exp\left[-\tfrac{1}{2} \sum_{\langle x,y \rangle} (\psi_x - \psi_y)^2 \right] \tag{17}$$

An improved quantity D_2 is defined analogously. Explicit results for $A_1^{(0)}$ and $A_2^{(0)}$ are given in Table 4 of ref. 15.

Obviously this modification does not affect the large-L behavior since $A_1^{(0)}(L) = A_1^{(0)}(\infty) + O(L^{-2})$. In the following we will see that the results for our largest lattice sizes are virtually unaffected by this kind of improvement. However, the benefit for the smaller lattices will be clearly visible.

4. DISCUSSION OF THE NUMERICAL RESULTS

First we simulated the BCSOS model at the roughening coupling $K_R = \frac{1}{2} \ln 2$ on square lattices of the size $L \times L$ with periodic boundary conditions imposed. We considered lattices with sizes ranging from $L = 8$ up to $L = 96$. The loop algorithm of Evertz *et al.*[22] enabled us to reduce the statistical error of the BCSOS data compared with those given in ref. 15 by a factor of about 5. We performed 4×10^6 measurements throughout, except for $L = 96$, where 3×10^6 measurements were performed. The number of loopupdates per measurement was 10 for $L = 8$, up to 35 for $L = 96$. This number was chosen such that the integrated autocorrelation times in units of measurements were about 1. These simulations took about 81 hr of CPU time on an IBM RISC System/6000 Model 590 (66 MHz) in total. The results for $l = 4$ for the critical BCSOS model are presented in Figs. 2–6. The numbers for the A's can be obtained from the authors on request.

Next we performed the simulations of the Ising model at the best-known value[16] $K_R = 0.4074$ for the roughening coupling. We used the modified cluster algorithm introduced in ref. 23. For a discussion of the algorithm see also ref. 24. The expectation values for K^l in the neighborhood of the simulation point are then obtained by reweighting.[26]

First of all we had to ensure that our results are not spoiled by a too small extension in the z direction. Obviously the thickness of the lattice has to be large compared to the width of the interface itself. It turns out that this requirement can be easily fulfilled since the width of the interface at K_R is smaller than 1 for the lattice size we will consider in the following.[7, 23, 9, 24]

In refs. 23–25 the dependence of interface properties on the extension of the lattice in the z direction was carefully checked. For couplings close to K_R and lattice sizes $L \leqslant 256$ it turned out that for about $L > 10$ no dependence on D can be detected within the obtained accuracy.

We performed an additional check for $L = 128$. We compared the interface width without bubbles for $D = 15$ and $D = 31$. We obtain $W_0^2 = 0.64647(25)$ for $D = 15$ and $W_0^2 = 0.64658(33)$ for $D = 31$. The definition of W_0^2 is given below.

Therefore we regard the extension $D = 31$ which we used throughout in the following simulations as perfectly safe.

Per measurement we performed five H-updates and five I-updates and in addition one metropolis sweep, where H and I refer to reflections at half-integer and integer z values, respectively. The number of updates per sweep was again chosen such that the integrated autocorrelation times in units of measurements are smaller than 1. The number of measurements was 100,000 for most of the lattice sizes. For $L = 48$, 192, and $L = 256$ we performed 93,500, 113,000 and 72,500 measurements, respectively. The total amount of CPU time used for the Ising simulations was about 63 days on an IBM RISC System/6000 Model 590 (66 MHz).

4.1. The Interface Width

Before discussing the results of the matching analysis, let us briefly study the behavior of the surface width, which was the basis of the Monte Carlo study of ref. 9. Following ref. 9, we define a normalized magnetization gradient as

$$\rho(z) = \frac{1}{2m_b L^2}\left[M\left(z+\frac{1}{2}\right) - M\left(z-\frac{1}{2}\right)\right] \tag{18}$$

where m_b is the bulk magnetization and M the total magnetization of a z slice of the lattice. Now the interface width is given by

$$W^2 = \left\langle \sum_z \rho(z)\, z^2 - \left(\sum_z \rho(z)\, z\right)^2 \right\rangle \tag{19}$$

We computed the interface width for the original configurations (W^2) and after removing the bubbles (W_0^2). In the rough phase of the Ising interface or an SOS model the surface width behaves like

$$W^2 = \text{const} + \frac{1}{2\pi\beta_{\text{eff}}} \ln L \tag{20}$$

for sufficiently large L. Here β_{eff} is determined by the point where the RG trajectory hits the x axis in the KT flow diagram. Therefore the slope of the curve at the roughening transition should be given by $1/\pi^2$. However, it was pointed out in refs. 15 and 10 that at the roughening transition corrections to this asymptotic behavior die out proportional to the fugacity (7), i.e., only proportional to the inverse of the logarithm of L. Hence these corrections cannot be neglected even for quite large lattice sizes.

To check this anticipated behavior we plot the surface thickness for the BCSOS model and the Ising interface with bubbles and bubbles removed in Fig. 1. For comparison two straight lines with slope $1/\pi^2$ are given. It turns out that even when our largest lattice sizes are considered, the slope is about 10% larger than the asymptotic one. Using therefore Eq. (20) with the slope $1/\pi^2$ as criterion to determine the roughening point leads to a considerably underestimation of the roughening temperature. Going to enormous lattice sizes such as $L = 960$ does not help that much to overcome the problem since the corrections die out only logarithmically in L.

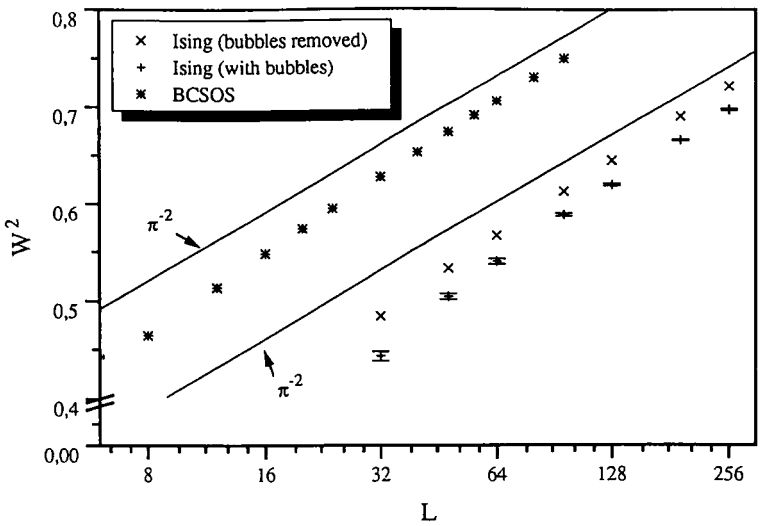

Fig. 1. Squared interface width W^2 plotted versus the lattice size L.

4.2. Matching Results

For the determination of the roughening temperature and the matching factor using the matching method we considered the four pairs of observables $(A_{1,2}, A_{3,2})$, $(A_{2,2}, A_{3,2})$, $(A_{1,4}, A_{3,4})$ and $(A_{2,4}, A_{3,4})$. In order to check the effect of removing the bubbles and the improvement by the continuous Gaussian model on our results we performed the whole analysis for the following four different choices of the observables:

(i) The bubbles being removed from the bulk phases, using the improved D_1 and D_2.

(ii) The bubbles being removed from the bulk phases, using A_1 and A_2.

(iii) Not removing the bubbles, using the improved D_1 and D_2.

(iv) Not removing the bubbles, using A_1 and A_2.

In all cases the statistical errors of the estimates for the roughening coupling and the matching factor were computed from a jackknife analysis put on top of the whole matching procedure.

The results for the roughening coupling K_R for the Ising interface based on (i) and (ii) are summarized in Table I. Using the improved quantities D_1

Table I. Results for the Roughening Coupling Obtained from Matching for Different Values of L and $l=2, 4$[a]

L	l	A_1	D_1	A_2	D_2
32	2	0.40602(15)	0.40727(14)	0.40657(16)	0.40831(21)
48	2	0.40648(16)	0.40716(16)	0.40678(17)	0.40760(21)
64	2	0.40675(14)	0.40722(14)	0.40692(15)	0.40735(18)
96	2	0.40719(14)	0.40741(15)	0.40727(16)	0.40745(17)
128	2	0.40733(15)	0.40748(16)	0.40734(19)	0.40748(21)
192	2	0.40762(14)	0.40768(14)	0.40762(15)	0.40766(16)
256	2	0.40748(14)	0.40751(14)	0.40762(16)	0.40765(16)
32	4	0.40529(10)	0.40678(9)	0.40589(10)	0.40740(10)
48	4	0.40610(9)	0.40709(8)	0.40647(9)	0.40748(9)
64	4	0.40649(8)	0.40728(8)	0.40677(9)	0.40750(9)
96	4	0.40702(8)	0.40745(8)	0.40717(8)	0.40754(9)
128	4	0.40727(7)	0.40752(7)	0.40733(8)	0.40755(9)
192	4	0.40753(7)	0.40766(7)	0.40754(7)	0.40764(8)
256	4	0.40738(7)	0.40745(7)	0.40741(7)	0.40746(7)

[a] For the matching $A_{3,l}$ together with either $A_{1,l}$, $D_{1,l}$, $A_{2,l}$, or $D_{2,l}$ are used. The bubbles in the Ising system are removed before the measurement.

Table II. Results for Matching Parameter b for Different Values of L and $l=2, 4$[a]

L	l	A_1	D_1	A_2	D_2
32	2	2.12(4)	2.68(5)	2.346(6)	3.14(11)
48	2	2.30(8)	2.74(12)	2.49(10)	3.05(16)
64	2	2.54(11)	2.92(12)	2.68(11)	3.02(16)
96	2	2.60(14)	2.84(18)	2.69(17)	2.88(20)
128	2	2.85(19)	3.05(23)	2.86(24)	3.05(29)
192	2	2.74(24)	2.82(27)	2.73(26)	2.80(28)
256	2	3.08(33)	3.15(35)	3.45(44)	3.54(48)
32	4	1.751(10)	2.048(11)	1.864(13)	2.194(18)
48	4	2.062(18)	2.419(22)	2.191(24)	2.548(28)
64	4	2.311(26)	2.703(32)	2.442(33)	2.816(42)
96	4	2.550(41)	2.87(6)	2.66(5)	2.95(7)
128	4	2.68(6)	2.91(7)	2.73(7)	2.94(8)
192	4	2.81(9)	2.96(10)	2.82(10)	2.94(11)
256	4	3.05(11)	3.16(12)	3.10(13)	3.19(13)

[a] For the matching $A_{3,l}$ together with either $A_{1,l}$, $D_{1,l}$, $A_{2,l}$, or $D_{2,l}$ are used. Bubbles are removed from the Ising configurations.

and D_2, we find that the results are consistent within two standard deviations starting from $L=96$ for $l=2$ as well as $l=4$. For our largest lattice size $L=256$ the difference of the results when using the unimproved observables A_1 and A_2 rather than D_1 and D_2 is smaller than the statistical error. However, looking at the results obtained from $L=32$ and $L=48$ makes it clear that a major part of the correction to scaling is eliminated by using D_1 and D_2 instead of A_1 and A_2.

In Table II we present the results for the matching factor B based on (i) and (ii). The observations are analogous to those for the roughening coupling.

For a blocksize $B \geqslant 32$ the results obtained from (iii) and (iv) are consistent within errorbars with those obtained from (i) and (ii). We therefore skip a detailed discussion of these results.

Following the above discussion, we regard the results for K_R and b obtained from (i) as the least affected by systematic errors. Therefore we take the weighted average of the results of (i) (i.e., the D_1 and D_2 columns of Tables I and II for $l=2$, $L \geqslant 96$, and $l=4$, $L \geqslant 128$ as our final result.

We obtain $K_R = 0.40754(5)$ and $B = 2.97(7)$. Computing the error-estimate, we have assumed that values obtained from the same simulation but from a different pair of observables are strongly correlated.

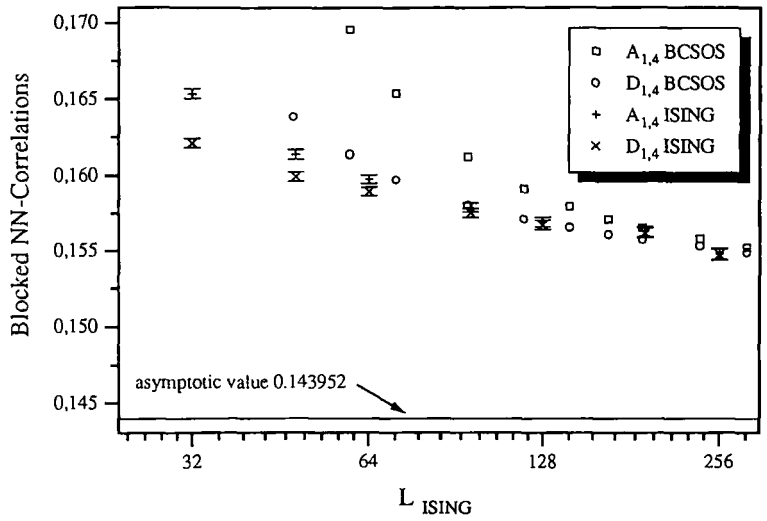

Fig. 2. $A_{1,4}$ and $D_{1,4}$ at the roughening transition as a function of $L^{\mathrm{I}} = bL^{\mathrm{S}}$ for the Ising interface as well as the BCSOS model.

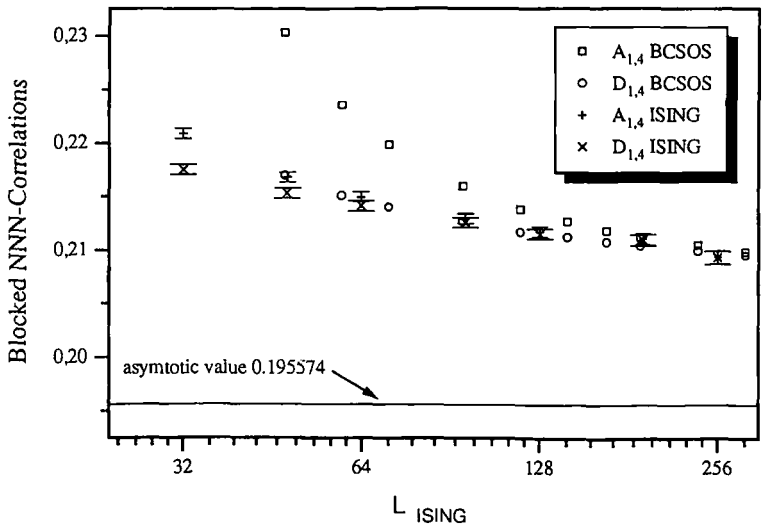

Fig. 3. $A_{2,4}$ and $D_{2,4}$ at the roughening transition as a function of $L^{\mathrm{I}} = bL^{\mathrm{S}}$ for the Ising interface as well as the BCSOS model.

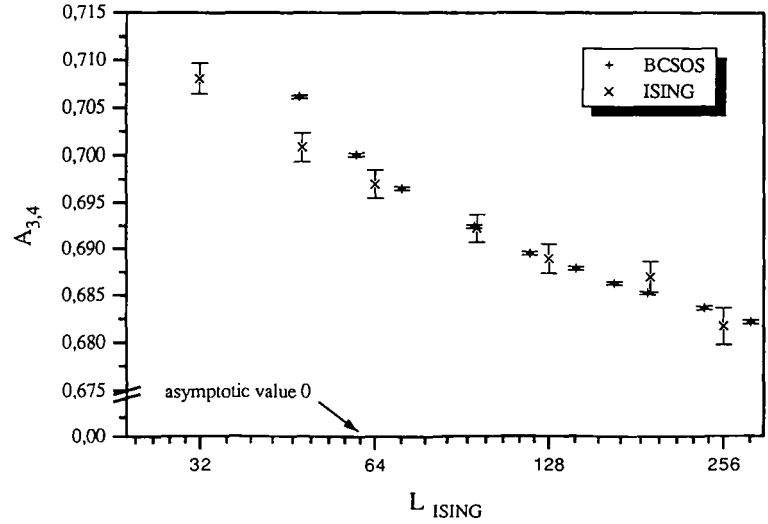

Fig. 4. $A_{3,4}$ at the roughening transition as a function of $L^{\mathrm{I}} = bL^{\mathrm{S}}$ for the Ising interface as well as the BCSOS model.

As an additional check of universality we plot all observables A_l considered for the critical BCSOS model as well also the Ising interface at $K_{\mathrm{R}} = 0.40754(5)$ as a function of L and L/b, respectively in Figs. 2–6.

Figure 2 shows the observables $A_{1,4}$ and $D_{1,4}$. The figure shows nicely the improvement gained by replacing $A_{1,4}$ by $D_{1,4}$. While the curves of $A_{1,4}$ for the Ising interface and the BCSOS model are only consistent for $L \leqslant 192$, the consistency extends down to at least $L = 96$ when $D_{1,4}$ is considered. For $A_{2,4}$ and $D_{2,4}$ given in Fig. 3 this improvement is visible even more drastically.

In the case of $A_{3,4}$ plotted in Fig. 4 the matching of the curves within the statistical accuracy sets in for $L^{\mathrm{I}} \geqslant 64$.

Figure 5 shows the observable $A_{4,4}$. This observable was not used for the determination of K_{R} and b. The fact that for $L^{\mathrm{I}} \geqslant 96$ the curves of $A_{4,4}$ for the Ising interface and the BCSOS model fall on top of each other strongly supports that the Ising interface and the BCSOS model have the same critical behavior. For $L^{\mathrm{I}} \geqslant 128$ also the curves of $A_{5,4}$ for the Ising interface and the BCSOS model become identical within error bars (Fig. 6).

Similar observations hold for $l = 1$ and $l = 2$. (The corresponding figures are not reproduced here.)

The matching program also allows to determine the nonuniversal constants appearing in formulas describing the divergence of observables

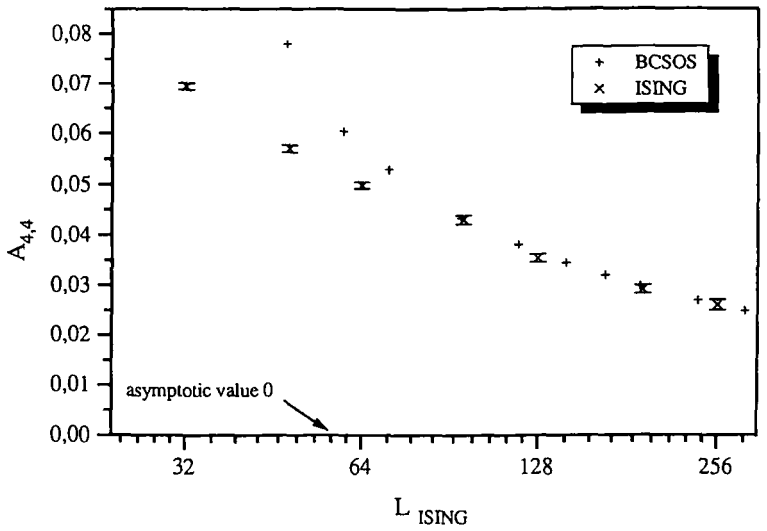

Fig. 5. $A_{4,4}$ at the roughening transition as a function of $L^1 = bL^S$ for the Ising interface as well as the BCSOS model.

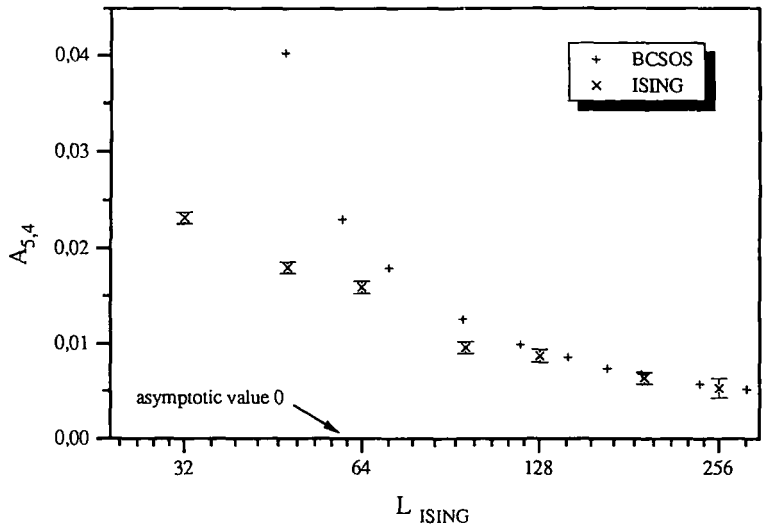

Fig. 6. $A_{5,4}$ at the roughening transition as a function of $L^1 = bL^S$ for the Ising interface as well as the BCSOS model.

near the roughening transition. The critical behavior of the correlation length ξ is described by[6]

$$\xi = A \exp(C\kappa^{-1/2}) \tag{21}$$

Along the lines of Section 5.3 of ref. 15, we obtain $A^{\mathrm{I}} = 0.74(2)$ and $C^{\mathrm{I}} = 1.03(2)$ for the Ising interface.

5. COMPARISON WITH OTHER STUDIES

Let us compare our result, $K_{\mathrm{R}} = 0.40754(5)$, with results obtained in previous Monte Carlo studies of the Ising interface.

We nicely confirm the value $K_{\mathrm{R}} = 0.4074(3)$ obtained by Hasenbusch[16] using similar methods as used in the present paper.

In a large-scale Monte Carlo simulation of lattices up to $960 \times 960 \times 26$ Mon *et al.*[9] studied the behavior of the interface width. They obtained $K_{\mathrm{R}}^{\mathrm{I}} = 0.409(4)$.

Mon *et al.*[8] determined the step free energy on lattices of size up to 96^3. They gave the estimate $T_{\mathrm{R}}/T_c = 0.54(2)$, which corresponds to $K_{\mathrm{R}} = 0.410(16)$.

Bürkner and Stauffer[7] obtained in their pioneering study $T_{\mathrm{R}}/T_c = 0.56(3)$, which corresponds to $K_{\mathrm{R}} = 0.396(22)$.

One should note that all these estimates are consistent within the quoted error bars with our present result.

It is also interesting to compare the Ising interface results with those obtained in ref. 15 for the ASOS model, $K_{\mathrm{R}}^{\mathrm{ASOS}} = 0.8061(3)$ and $b_m^{\mathrm{ASOS}} = 2.8(3)$. In the low-temperature limit the ASOS coupling and that of the Ising model are related as $K^{\mathrm{I}} = \frac{1}{2}K^{\mathrm{ASOS}}$. At finite temperatures one expects that the bubbles and the overhangs disorder the Ising interface compared to the ASOS model. Hence one expects the roughening transition of the Ising interface to occur at a lower temperature than for the ASOS model and indeed $K_{\mathrm{R}}^{\mathrm{I}} - \frac{1}{2}K_{\mathrm{R}}^{\mathrm{ASOS}} = 0.0044\ (2)$.

Such a shift was already predicted by low-temperature expansions[27] $K_{\mathrm{R,\,LT}}^{\mathrm{I}} = 0.404(12)$ and $K_{\mathrm{R,\,LT}}^{\mathrm{ASOS}} = 0.787(24)$. However, one should note that the difference of these two results is smaller than the given error bars. The matching factors for the two models are equal within the quoted error bars. The direct matching of the Ising interface with the ASOS model performed in ref. 16 gives the more precise result $b_m^{\mathrm{I}}/b_m^{\mathrm{ASOS}} = 1.17(4)$ for this particular comparison.

6. CONCLUSION AND OUTLOOK

Using the finite-size scaling method of ref. 15, we unambigously demonstrated the KT nature of the roughening transition in the (001)

interface of the 3D Ising model. Our estimate for the inverse of the roughening temperature $K_R = 0.40754(5)$ is almost a factor of 100 more accurate than the best previously published value.[9]

Previous studies have been mainly plagued by logarithmic corrections at the roughening transition. This problem has been overcome completely.

In addition, the use of efficient, virtually slowing-down-free cluster algorithms for the BCSOS model[22] and the Ising interface[23,24] allowed us to generate more than 10^6 independent configurations in the case of the BCSOS model and about 10^5 independent configurations for the Ising model for all lattice sizes using about 2 months of CPU time on an IBM RISC System/6000 Model 590 (66 MHz).

This high statistical accuracy can be further improved, first, simply by using more CPU time and, secondly further improving the implementation of the algorithm.

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