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Interface roughening in the three-dimensional Ising model

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Using Monte Carlo simulations, we determine the roughening temperature of a (100) interface in the three-dimensional Ising model to be at about 0.542±0.005 in units of the critical temperature. For higher temperatures, the squared interface thickness is found to increase logarithmically with system size. These results agree well with theoretical predictions as well as previous numerical determinations.

In three dimensions, a two-dimensional liquid-vapor interface has a finite thickness W which diverges logarithmically if the area of this interface goes to infinity.[1] In the lattice-gas approximation (Ising model), this roughening is seen only above some roughening temperature T_R. Previous Monte Carlo simulations[2,3] found a ratio T_R/T_c of 0.56±0.03 and 0.54±0.02, and series expansions[4] gave 0.55±0.02. While that agreement is satisfactory, it is not impressive since a very simple approximation identifies the roughening transition with that of the two-dimensional lattice gas and then gives 0.503 for this ratio, using the known Curie temperatures[5] of square and simple cubic lattices. Thus, the estimates for the deviation from this trivial approximation vary appreciably, if one also considers the maximum values that lie within the error bars.

Therefore, the present paper tries to reexamine the oldest of these estimates[2] using the same definitions but larger lattices simulated over longer times on a better computer (ETA 10Q and Cyber 205) with a vectorized multispin coding program (64 spins per word).[6] As in Ref. 2, we used a simple cubic lattice of size $L\times L\times 26$, with periodic boundaries in horizontal directions, i.e., parallel to the $L\times L$ initial interface, with L now up to 960 instead of 300. Also, boundary effects were reduced by antiperiodic instead of fixed boundary conditions at the top and bottom. That means the uppermost plane was regarded as the lower neighbor of the lowermost plane after all its spins were reversed. Thus, interface motion was less restricted and the full height of the lattice could be used to study the interface profile; fixed boundaries as in Ref. 2 make the top layers and the bottom layers near the boundary quite useless.

We used a vectorized[6] shift-register random number generator with an array of 250 (Cyber 205) or 1279 (ETA) random integers. The next integer is then produced by a bit-per-bit exclusive—or of integers 1 and 148 for the short array and of integers of elements 1 and 217 for the long array on the ETA, after which the first integer element is omitted from the array and the new integer is added to it. (The longer array was needed on the faster ETA since otherwise the vectorization caused problems.)

As in Ref. 3, we reached a speed of about 40 million Monte Carlo steps per second and per processor (slightly slower on the Cyber 205). Up to eight runs with typically 40 000 Monte Carlo steps (MCS) per site were made to ensure thermal equilibrium in this kinetic Glauber model; the interface thickness fluctuated with a characteristic time of order 10^4 MCS. (For $L=512$ and $T/T_c=0.56$ we made one run up to 200 000 MCS but found no long-time trends.)

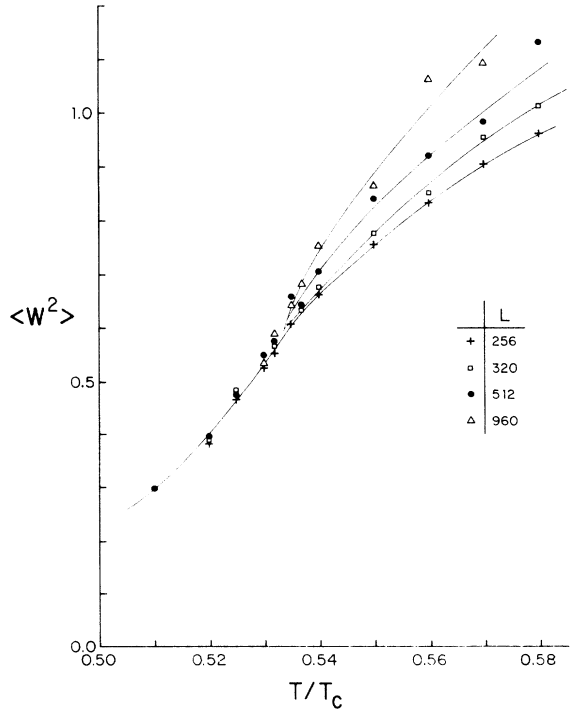

FIG. 1. Variation of squared width vs T/T_c for various L.

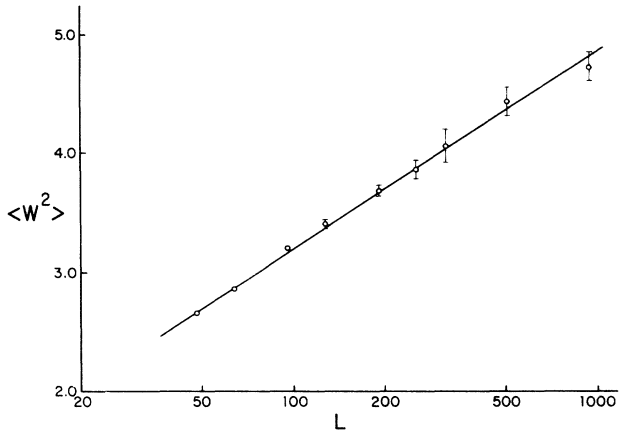

FIG. 2. Squared width vs $\ln(L)$ at $T/T_c=0.8$.

We primarily used the standard definition[7] of the width W even though fits by error functions might be better:[8] The magnetization profile $M(z)$ was determined for each plane at height z parallel to the initial interface. The normalized gradient is

$$g(z)=[M(z+1)-M(z)]/[M(26)-M(1)] .$$

The average position $\langle z\rangle$ of the interface is determined as the integral over $z\,g(z)$ and the average squared position $\langle z^2\rangle$ as the integral over $z^2\,g(z)$. Then the squared width is $W^2=\langle z^2\rangle-\langle z\rangle^2$. We also used a different definition of W as the integral over $[M_0-|M(z)|]/M_0$ where M_0 is the positive spontaneous magnetization; results and fluctuations for these two definitions were comparable.

Figure 1 shows the squared width (standard definition[2,7]) versus T/T_c for different linear dimensions L. While for temperatures below about $0.53T_c$ different L give the same width, the results branch out for T/T_c above about 0.54. Far above this transition, at

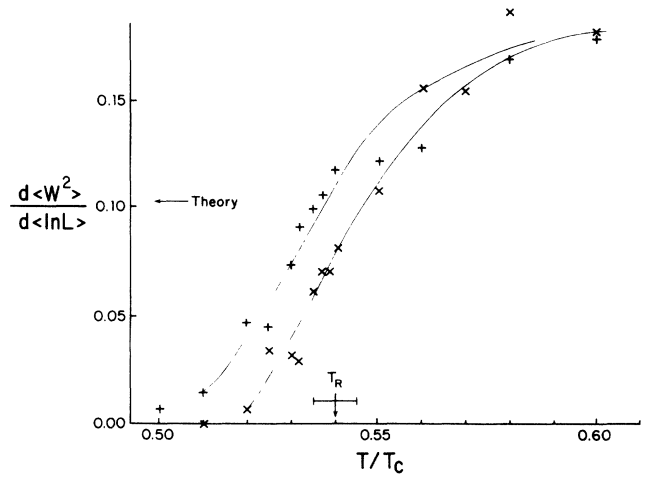

FIG. 3. Roughening amplitude vs temperature; the roughening amplitude is determined as the slope of W^2 vs $\ln(L)$. (+) fits for $32\le L\le 96$, (×) fits for $96\le L\le 960$.

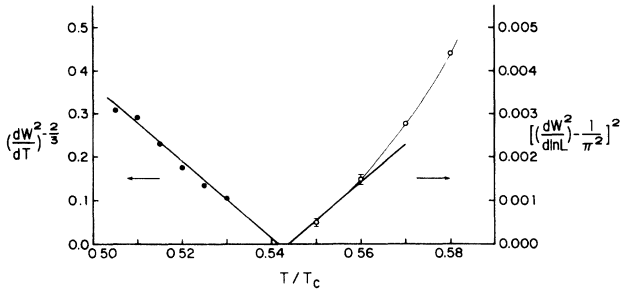

FIG. 4. Test of Kosterlitz-Thouless theory: $(dW^2/dT)^{-2/3}$ vs T/T_c [left scale, Eq. 1(a)] and $[dW^2/d\ln L)-1/\pi^2]^2$ vs T/T_c [right scale, Eq. 1(b)]. The theory predicts straight lines asymptotically.

$T/T_c=0.8$, a plot of W^2 versus $\ln L$ (Fig. 2) gives a good straight line. (Similar behavior was found near $T/T_c=0.6$.) For percolation, W instead of W^2 was found[9] to vary as $\ln L$; such a law agrees less well with our present data but cannot be excluded. Figure 3 shows the slope of W^2 versus $\ln L$ as a function of temperature for two size ranges. Again, these slopes vary drastically near $T/T_c=0.54$. We cannot determine whether a jump actually occurs in the infinite system, but if it does it is consistent with the Kosterlitz-Thouless value (arrow in Fig. 3). Effective roughening temperatures can be identified with the inflection points in these curves; from these we estimate $T_R/T_c=0.540\pm0.005$ for infinite systems. If we analyze our data assuming Kosterlitz-Thouless theory[10] to be true,

$$W^2\propto \text{const}+(T_R-T)^{-1/2}$$

for $T<T_R$, and

$$W^2/\ln(L)=\pi^{-2}+\text{const}(T-T_R)^{1/2}$$

for $T>T_R$, we find reasonable agreement, Fig. 4, for $T_R/T_c=0.543\pm0.003$.

Our final estimate (i.e., using all information but emphasizing Fig. 4)

$$T_R/T_c=0.542\pm0.005$$

is consistent with earlier results and shows that their relatively large error bars were realistic. (We note that our calculations used much more than one hundred times the number of spin flips compared with Burkner.[2]) In absolute units this corresponds to $kT_R/J=2.445$. The variation with $\ln L$ is compatible with the logarithmic growth law, $W\propto\ln(t)$, for not too long times in three dimension.[8] These data are also compatible with $W\propto t^{0.08}$.

Although our asymptotic value of $W^2/\ln(L)$ is compatible with the prediction $0.1(=1/\pi^2)$ at the roughening transition for models with a well-defined local interface position,[10] the power-law behavior above T_R is less well supported.

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