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Surface Tension and Universality in the Three-Dimensional Ising Model

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The amplitude τ_0 of the interfacial free energy per unit area (or surface tension) of the body-centered-cubic Ising model is found using a direct monte carlo simulation technique. The combination $\tau\xi^2/k_B T_c$, where ξ is the correlation length, is shown to agree within the precision of the simulations with a previously reported estimate for the simple cubic lattice. Evidence is also presented for the universality of the finite-size scaling amplitude for the surface tension.

KEY WORDS: Surface tension; universality; Ising models; Monte Carlo simulation; finite size scaling; liquid–vapor interfaces.

1. INTRODUCTION

Universality provides the framework for a detailed description of the singular behavior of complex physical systems. For if universality holds, one may consider simplified models which are allegedly in the same universality class as the complex ones. Assumptions of universality are usually tested by careful measurements, on a variety of systems, of critical exponents and various combinations of critical amplitudes which are supposed to be universal. These may be compared to like quantities computed for the simplified models.

A number of amplitude ratios involving the surface tension have been proposed as universal.[2] Although early measurements and computations exhibited sizeable disagreements between theory and experiment,[(2)] more recent computations[(3)] and a synthesis of available experimental infor-

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[2] For a recent review see Ref. 1.

mation by Moldover[4] are in much closer accord. However, significant differences on the order of 30% remain between experiments on fluid systems and results of three-dimensional Ising Monte Carlo simulations.[3]

In this paper we have extended the techniques and refined the Ising lattice simulations in three significant ways. First, antiperiodic boundary conditions (in one direction) have been used to induce an interface, in contrast to previous simulations with spins at the boundary layers fixed up or down.[5,3] Such a change should be a test of the numerical methods, since both boundary conditions should serve equally well. Second, a different lattice, namely, the bcc, has been used to check at least if the methods show universality among Ising systems. Finally, a larger-scale simulation than previously reported has also been used. In addition the finite-size scaling amplitude of the surface tension at the bulk critical point has been calculated for both the sc and bcc lattices to test the hypothesis of universality of such amplitudes.

We have found that within the statistical errors, the results are independent of the boundary conditions described above, and the universal ratio involving surface tension and correlation length is the same for both the sc and bcc systems. Finally, for the first time, evidence is provided that the finite-size scaling amplitude for the surface tension is universal.

The remainder of this paper is divided as follows. In the next section notation is defined and particular amplitudes are specified. The method used in the present simulations is presented. In Section 3 results are presented, while Section 4 is reserved for concluding remarks.

2. NOTATION AND DEFINITIONS

The bcc lattice is considered as a sc lattice with a two point basis. The nearest-neighbor Ising system is then composed of two interpenetrating sublattices, each containing $N \times N \times N$ sites. As usual the reduced temperature is given by $t = (T_c - T)/T_c$.

The surface tension $\tau(N, t)$ is given by

$$\tau(N, t) = \frac{1}{N^{d-1}} \left[F_{\mathrm{ap}}(N, t) - F_{\mathrm{p}}(N, t)\right] \tag{2.1}$$

where $F_{\mathrm{p}}(N, t)$ is the free energy of the lattice of $2N^d$ sites with periodic boundary conditions in all d directions. Similarly, $F_{\mathrm{ap}}(N, t)$ is the free energy for the system of $2N^d$ sites with periodic boundary conditions in $d-1$ dimensions and antiperiodic boundary conditions in one direction. At low temperatures such conditions will produce an interface. The scheme is implemented by coupling the spins on one face with spins on the opposite face with coupling constant $(-J)$. The other faces have spins coupled with appropriate partners with coupling constant $(+J)$ as in the case of ordinary periodic boundary conditions. The situation is shown schematically in Fig. 1. This method has the advantage that there are no walls or boundaries which pin the spins up or down. In the latter case it is assumed[5,3] that the boundary energy cancels, but the effect may contribute to slow convergence toward the scaling limit from which one obtains the amplitude for the interfacial tension. The method of introducing a layer of antiferromagnetic bonds (the "seam" method) is originally due to Onsager.[6] In (2.1) the infinite N limit must be taken to give the proper interfacial free energy.

In the calculation one considers, as in the earlier simulations,[5,3] the ratio of partition functions,

$$\ln \frac{Z_{\mathrm{ap}}}{Z_{\mathrm{p}}} \tag{2.2}$$

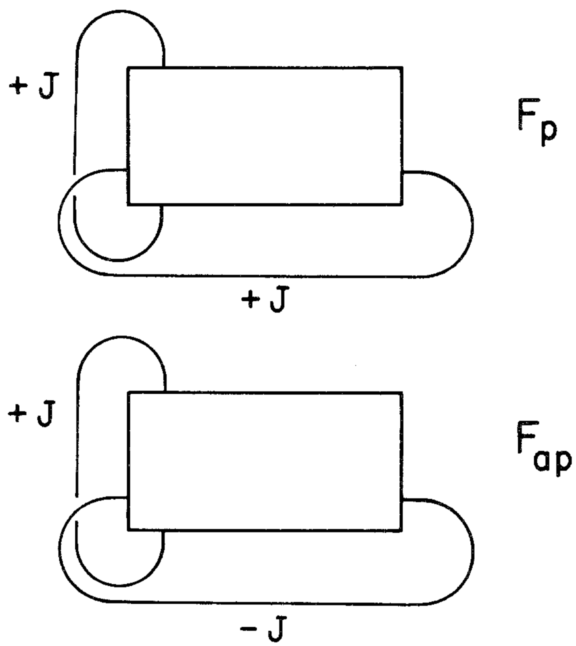

Fig. 1. Schematic illustration of the boundary conditions used to generate the two free energies.

Furthermore a multistage sampling, indicated schematically by

$$\frac{Z_{\text{ap}}}{Z_{\text{p}}} = \frac{Z_{\text{ap}}}{Z_1} \cdot \frac{Z_1}{Z_2} \cdots \frac{Z_n}{Z_{\text{p}}} \tag{2.3}$$

has been used. The intermediate stages, $Z_1, Z_2,...$ are generated by Hamiltonians $H_1, H_2,...$ which interpolate between H_{ap} and H_{p}. In the present simulation up to seven intermediate stages have been used (five more than in the sc analysis.)

The interpolating Hamiltonians H_i have been constructed by letting the bonds which couple the first layer to the last layer be J_i, with $-J < J_1 < J_2 \cdots < J$. The set of J_i were chosen for computational convenience and for the bulk of the calculations five intermediate stages were used with $[J_i] = [-0.6J, -0.3J, 0.0, 3J, 0.6J]$. About 10^5 Monte Carlo steps per spin were sampled for each stage.

3. RESULTS

In Fig. 2 the quantity $\tau(N, t)\, N^{\mu/\nu}$ versus $N^{\mu/\nu} t^{\mu}$ is plotted for the bcc lattice with up to and including $N = 8$ cells on each edge. The finite-size scaling assumption for the surface tension is taken to be[5,3]

$$\tau(N, t) = \tau_0 t^{\mu} \Sigma(N^{1/\nu} t) \tag{3.1}$$

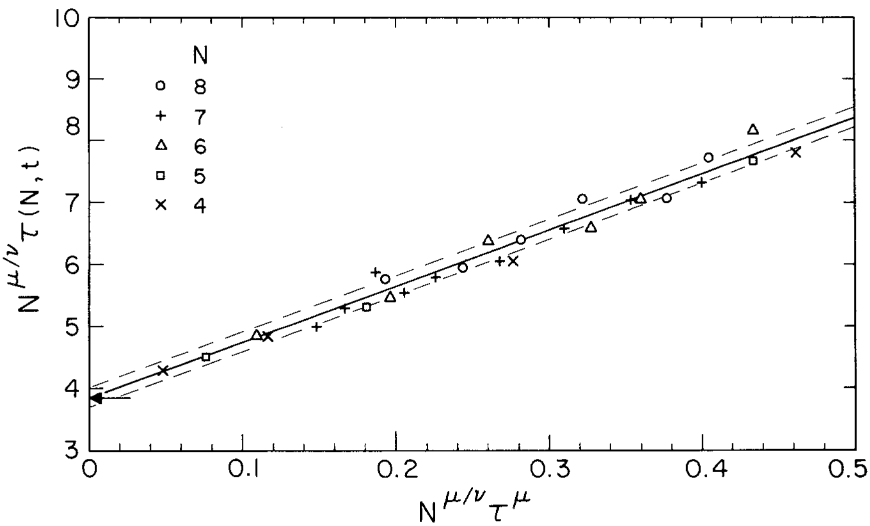

Fig. 2. $N^{\mu/\nu}\tau(N, t)$ versus $x^{\mu} = N^{\mu/\nu} t^{\mu}$ for a variety of temperatures and system sizes $4 \leqslant N \leqslant 8$. The finite-size scaling assumption suggests that for sufficiently large x^{μ} the curve should be linear with slope $\tau_0/k_B T_c$.

where τ_0 is the infinite-system amplitude for the interfacial tension. The behavior of the scaling function has been discussed in the references noted. The scaling function has the limits $\Sigma(x \to 0) \sim x^{-\mu}$ and $\Sigma(x \to \infty) = 1$. Note from the limiting forms that the slope of the line in the large $x^\mu = N^{\mu/\nu} t^\mu$ limit in Fig. 2 yields τ_0.

Apparently the linear region is reached rather quickly. The same sort of behavior was observed in the case of the two-dimensional Ising model.[5] Deviations from linearity are, however, seen for small N. Although there is no certainty that the asymptotic regime has been reached, the observed linearity indicates that the scaling function Σ may have a simple form as was suggested in the two-dimensional case.

From the figure, it is observed that 75% of the points lie within a band of slope 9.12 ± 0.6, which yields the estimate $\tau_0/k_B T_c = 1.435 + 0.09$. The value $1/k_B T_c = 0.15737$[7] has been used, along with the value $\mu = (d-1)\,\nu = 2\nu = 2(0.63)$.[8]

In Fig. 3, the quantity $N^{\mu/\nu}\tau(N, 0)/k_B T_c$ versus $N^{\mu/\nu}$ has been plotted for both the bcc and sc lattices. Note the sc data using the "seam" method are new. Data reported earlier[3] employed different boundary conditions.

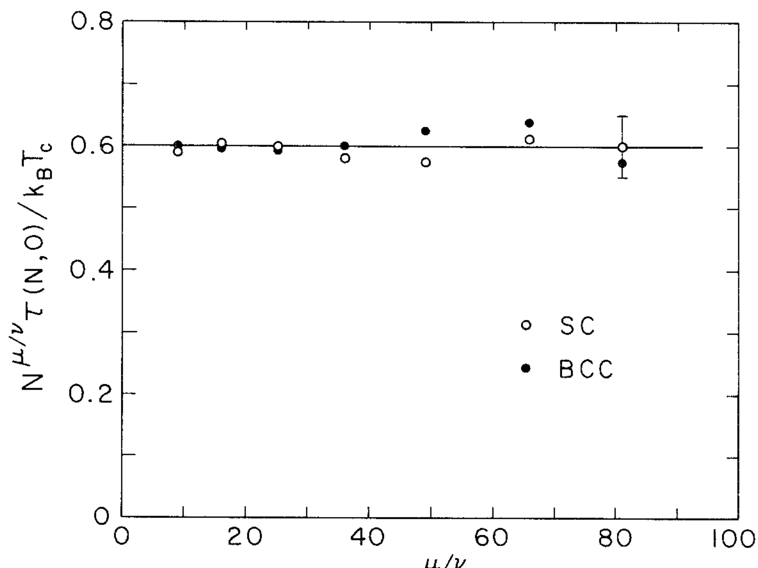

Fig. 3. $N^{\mu/\nu}\tau(N, 0)/k_B T_c$ versus $N^{\mu/\nu}$ for the bcc and sc lattices. In the scaling limit, the former quantity should approach a constant f_0.

From the form of the scaling given in Eq. (2.1) and the limiting behavior of the function Σ, one has

$$\frac{\tau(N,0)}{k_B T_c} \approx f_0 N^{-(d-1)} \tag{3.2}$$

Note the hyperscaling assumption $(d-1)\nu = \mu$ has been made throughout and also that f_0 has the interpretation of the *total* excess interfacial free energy normalized by $k_B T_c$. One may conjecture that the finite-size scaling amplitude f_0 is universal in analogy with the proposal by Privman and Fisher[9] that the finite-size amplitude for the singular part of the free energy is universal. If the amplitude is indeed universal, the curves should coincide without further adjustment. Inspection of Fig. 3 shows the results for the two lattices are quite close even though estimates for $\tau_0/k_B T_c$ differ by about 20%. The arrow in Fig. 2 shows the bcc data point at $t=0$ using the finite size amplitude $f_0 \simeq 0.6$ from Fig. 3.

4. DISCUSSION

In this short paper we have reported the results of Monte Carlo simulations of the surface tension of the bcc Ising system. The results are particularly timely because of a recent synthesis of experimental data by Moldover[4] and their relation to a previous Monte Carlo estimate based on the Ising sc lattice.[3] Moldover examined the values for a selection of fluids of the allegedly universal ratio $\tau\xi^{d-1}/k_B T_c$, where τ is the surface tension and ξ the correlation length. The confluence of the experimental data appears to differ by about 30% from the sc Monte Carlo data reported previously.[3] Hence it was necessary to test the universality of the simulations.

The results reported here and summarized in Table I appear to confirm the universality. The correlation length amplitudes $(T > T_c)$ for the sc and bcc lattices are from series analyses of Tarko and Fisher.[10] The estimates for $\tau_0/k_B T_c$ for the two lattices differ by about 20%, but the universal ratios differ by considerably less. Of course this close agreement may be fortuitous since our simulations suggest a (very cautious) 10% confidence in the surface tension amplitudes themselves. Furthermore there is, as always, the possibility that larger systems need to be considered to see the proper asymptotic scaling behavior.

Our method has been arranged to avoid some systematic problems by using the "seam" boundary conditions for the bcc. Furthermore, because of the added interest, the simulations for the bcc have been more extensive than those originally reported for the sc.[3] The difference between fluid data and the Ising simulations remains unexplained.

Table I. Summary of Results and Comparison to Experiments

	$f_1^{-\,a}$	$f_1^{+\,a}$	$\tau_0/k_B T_c$	$\frac{\tau_0(f_1^+)^2}{k_B T_c}$
sc	0.244 $+.001$	0.47826 $\pm.0004$	1.2 ± 0.1[b]	0.27 $\pm.023$
bcc	0.227 $\pm.005$	0.44456 $\pm.0004$	$1.435 \pm .09$	0.284 $\pm.018$
Fluids				0.386[c]

[a] Correlation length amplitudes above and below T_c from Ref. 10.
[b] Reference 3.
[c] Reference 4, median fluid.

Evidence has also been presented for the universality of the finite-size scaling amplitude at bulk criticality. Privman and Fisher[(9)] presented arguments for the universality of the finite-size amplitude of the bulk *free energy*. Such hypothesis has been tested in Ising simulations by Mon[(11)] and shown to hold within the numerical precision. If the finite-size amplitude of the surface tension is indeed universal, it suggests the arguments (in which the system size plays a special role as a scaling field) can be extended to beyond-the-bulk free energy contributions. This would be consistent with similar results for the excess free energy of free surfaces.[(12)] These possibilities require further consideration.

ACKNOWLEDGMENTS

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REFERENCES

1. K. Binder in *Phase Transitions and Critical Phenomena*, C. Domb and J. L. Lebowitz, eds. (Academic, New York, 1983); also see David Jasnow, Critical phenomena at interfaces, *Rep. Prog. Phys.* **47**:1059 (1984).
2. K. Binder, *Phys. Rev. A* **25**:1699 (1982).
3. K. K. Mon and D. Jasnow, *Phys. Rev. A* **31**:4008 (1985).
4. M. R. Moldover, *Phys. Rev. A* **31**:1022 (1985).
5. K. K. Mon and D. Jasnow, *Phys. Rev. A* **30**:670 (1984).
6. L. Onsager, *Phys. Rev.* **65**:117 (1944).
7. M. J. George and J. J. Rehr, *Phys. Rev. Lett.* **53**:2063 (1984).

8. J. C. LeGuillou and J. Zinn-Justin, *Phys. Rev. B* **21**:3976 (1980).
9. V. Privman and M. E. Fisher, *Phys. Rev. B* **30**:322 (1984); see also M. P. Nightingale and H. W. J. Blöte, *J. Phys.* **A16**:L657 (1983) and J. L. Cardy, *J. Phys.* **A17**:L385 (1984).
10. H. B. Tarko and M. E. Fisher, *Phys. Rev. B* **11**:1217 (1975).
11. K. K. Mon, *Phys. Rev. Lett.* **54**: 2671 (1985).
12. K. K. Mon and M. P. Nightingale, *Phys. Rev. B* **31**:6137 (1985).