Latent heat of the fcc Ising antiferromagnet

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(Presented on 10 January 2007; received 26 October 2006; accepted 16 November 2006; published online 21 March 2007)

To obtain critical parameters of the fcc Ising antiferromagnet from Monte Carlo data, a numerical estimate of the latent heat Δ is required. The precision of current estimates is about 3%, and ultimately limits the precision achieved for the disordered state at the Néel temperature T_N. Here we make several different estimates of the latent heat, using finite size scaling of Monte Carlo data, and show that a superior method yields a 25-fold improvement [$\Delta=0.4559(6)$] in comparison with our older result [$\Delta=0.455(15)$]. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2693929]

The nearest neighbor fcc Ising antiferromagnet undergoes a first order phase transition[1–5] at the Néel temperature, T_N. The model is usually invoked to explain the phase diagrams of binary alloys such as CuAu and FePt. A variety of techniques has been employed to study the model, including mean field theory,[1] series expansions,[2] and Monte Carlo simulation.[3–5] Monte Carlo simulations have provided the most precise estimates for the critical parameters,[5] and these results are in fair to good agreement with those obtained from series expansions.[2,5] In particular, at T_N, the internal energy and entropy of the ordered state—which coexists with a disordered state—are known with a precision comparable to those of the fcc Ising ferromagnetic model[5] (about a part in 10 000). Estimates of the critical parameters for the disordered state, however, are not nearly as precise, a problem entirely attributable to the difficulty of obtaining the latent heat of the infinite crystal from Monte Carlo simulations on finite systems. Here we present a much improved finite size scaling analysis of our Monte Carlo data which provides a more precise estimate of the latent heat.

The fcc Ising antiferromagnet describes a simple binary alloy which at low temperatures forms a superlattice. The Hamiltonian is $H=-J\Sigma_{\langle i,j\rangle}S_iS_j$ where the sum is over all pairs of nearest neighbor Ising spins ($S_i=\pm 1$). The spins reside on the vertices of a three dimensional fcc lattice with periodic boundary conditions containing $N=4L^3$ spins, where L is the linear dimension of the fcc lattice. The ground state of the antiferromagnetic model (with $J=-1$) is infinitely degenerate due to spin frustration and consists of an uncorrelated stack of antiferromagnetic (AF) ordered planes.[6] At finite temperature the degeneracy is lifted by thermal fluctuations, known as the order-by-disorder effect, which select those ground states which possess alternating ferromagnetic (FM) ordered planes,[7] perpendicular to the AF order.

Since the phase transition at T_N is first order, hysteresis is often experienced during Monte Carlo simulations[3,4] making it difficult to obtain a precise estimate of the transition temperature and critical parameters. In recent years, the emergence of flat histogram Monte Carlo techniques[8] has provided an ideal method by which to study first order transitions since hysteresis is completely removed. The technique, described elsewhere,[5,8] yields the density of states, $g(E/J)$, from which thermodynamic functions can readily be calculated at all temperatures for both the FM and AF models simultaneously. The analysis presented here is a reanalysis of the data used in our Ref. 5, and where mathematical definitions and simulation details can be found.

The key numerical results from our recent study[5] are listed in Table I for the free energy/site (f), internal energy/site ($u_\pm$), and the entropy/site ($s_\pm$) at T_N, where "+" and "−" refer to the disordered (high T) and ordered (low T) states, respectively. It is clear that the results for the disordered state are not nearly so precise as those for the ordered state. The reason for the difference is simple: For the model studied, $T_N(L)>T_N(\infty)$ and so our estimates of the internal energy and entropy at $T_N(\infty)$ are those of the ordered state, u_- and s_-, respectively. To obtain u_+ and s_+ we require an estimate of the latent heat Δ, since $\Delta=u_+-u_-$ while the entropy is obtained via $f=u_\pm-Ts_\pm$.

The delta function peak in the heat capacity/site (c) at T_N for the infinite crystal is both rounded and shifted for the finite crystal, and to an excellent approximation the peak is Gaussian. Our original estimate of the latent heat,[5] $\Delta=0.455(15)$, was obtained from the scaling of the peak height and inverse half width of c. A temperature dependent background also contributes to c, but this contribution is of the order unity while the peak height diverges as L^d, where d is the dimension of the lattice. Fits of c to a Gaussian (see Ref. 5 for details) are shown in Fig. 1 for $L=12$, 16, 20, and 24.

TABLE I. A comparison of our old and revised estimates of the critical parameters at $T_N=1.7217$.

	Old estimates	Revised estimates
f	−2.028 09(4)	−2.028 09(4)
u_+	−1.354(15)	−1.353 35(62)
u_-	−1.809 25(15)	−1.809 25(15)
s_+	0.391(6)	0.391 85(39)
s_-	0.127 11(11)	0.127 11(11)
T_N	1.721 7(8)	1.721 7(8)

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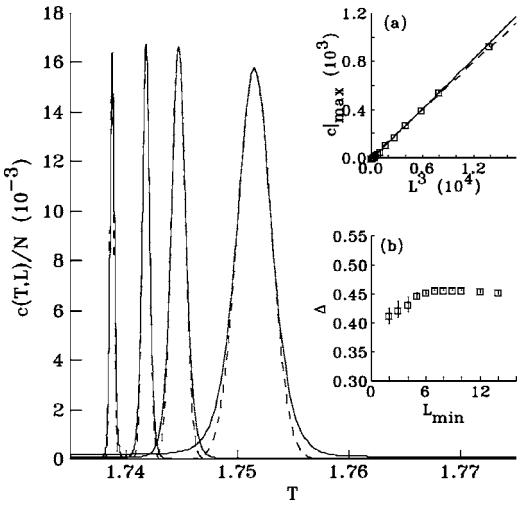

FIG. 1. Heat capacity/site divided by N for $L=12,16,20$, and 24 (solid line). Gaussian fits (dashed lines). Inset (a) show the peak height, $c|_{\max}$ diverging as L^3. The dashed line is a fit to Eq. (1) while the solid line is a fit to Eq. (7). Inset (b) shows the value of Δ obtained from fits to Eq. (7), where $L_{\min}$ is the smallest system size used, which becomes constant for $L>6$.

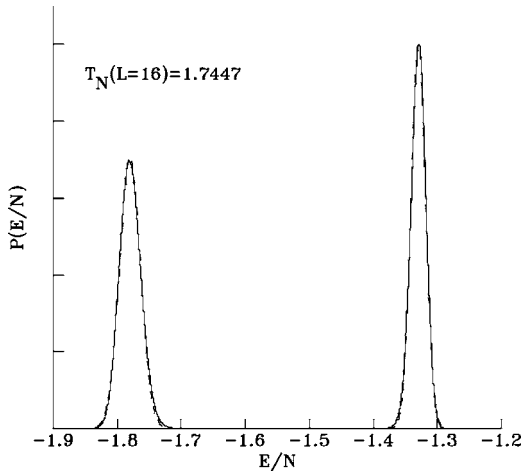

FIG. 2. Probability distribution of states with energy E/N, $P(E/N)$, for $L=16$ at $T_N(L=16)=1.7447$, the temperature for which c is maximal (solid line). The solid line is simply $P(E)=g(E)e^{-\beta E}$. Double Gaussian fit also shown (dashed line).

The agreement with the Gaussian form becomes better as L increases, the difference being of the order of the background.

For a first order transition,[9] the peak height, $c|_{\max}$, should diverge with increasing L as L^d. To take into account the background, we fit the peak height $c|_{\max}(L)$ to the form

$$c|_{\max}(L) = c_0 + c_3 L^3 \tag{1}$$

and similarly, the inverse half width, $\Gamma(L)$,

$$\Gamma(L) = \Gamma_0 + \Gamma_3 L^3, \tag{2}$$

so that in the limit of large L, $\Delta=\sqrt{2\pi}c_3/\Gamma_3$. The fit to Eq. (1) is shown in Fig. 1(a) and $c_0=3(6)$ is of the expected order. An obvious failure of this method is that the L and T dependences of the background have been ignored, and the latent heat determined by this method may be biased by these omissions. However, as we shall show, the term c_0 has a mathematical origin and must be present even if the background could be subtracted from the data perfectly.

For a first order transition with L large, the probability distribution of states with energy/site ϵ, $P(\epsilon)$, is simply the sum of two Gaussians[10] centered about the mean energy/site of the disordered and ordered states, $u_\pm$. In Fig. 2 we show the characteristic $P(\epsilon)$ for $L=16$ at $T_N(L=16)=1.7447$. The form of $P(\epsilon)$ suggests a better method for extracting Δ.

First we write the probability as

$$P(\epsilon) = \frac{w_+}{\sqrt{2\pi\sigma_+^2}} e^{-1/2((\epsilon-u_+)/\sigma_+)^2} + \frac{w_-}{\sqrt{2\pi\sigma_-^2}} e^{-1/2((\epsilon-u_-)/\sigma_-)^2}, \tag{3}$$

where $w_\pm$ are, for finite systems, smooth functions of temperature weighting the contribution from the disordered and ordered states. Clearly, $w_+ + w_- = 1$, and $w_\pm \geqslant 0$. For the infinite crystal w_+ is the Heaviside function, $w(T)=\Theta(T-T_N)$, since the transition is sharp. The heat capacity/site of the ordered and disordered states is simply $c_\pm = N\beta^2\sigma_\pm^2$, while the total heat capacity is

$$c = w_+ c_+ + w_- c_- + N\beta^2 w_+ w_- [u_+ - u_-]^2. \tag{4}$$

In the case where $u_\pm$ and $\sigma_\pm$ are slowly varying functions of T, Eq. (5) predicts that c is a maximum when $w_+ = w_- = \frac{1}{2}$, which we have confirmed to a precision better than 1%. Thus we have

$$c|_{\max}(L) = \frac{1}{2}[c_+(L) + c_-(L)] + \left[\frac{\Delta(L)}{T_N(L)}\right]^2 L^3, \tag{5}$$

where Δ, $c_\pm$, and T_N may all possess a size dependence. If we assume for the moment that Δ and $c_\pm$ are independent of L at $T_N(L)$, then the substitution $T_N(L)=T_N(\infty)+aL^{-1}$ (see Ref. 5) yields

$$c|_{\max} = c_0 + \left(\frac{\Delta}{T_N}\right)^2 L^3 [1 + 2a(T_N L)^{-1} + a^2 (T_N L)^{-2}]^{-2}. \tag{6}$$

A Taylor expansion of the term in square brackets (valid since $a \ll T_N L$) gives

$$c|_{\max} = \hat{c}_0 + \hat{c}_1 L^1 + \hat{c}_2 L^2 + \hat{c}_3 L^3, \tag{7}$$

(where we have neglected nondivergent terms but retained the constant $\hat{c}_0$) with

$$\hat{c}_0 = \frac{1}{2}(c_+ + c_-) - 20a^3\Delta^2 T_N^{-5},$$

$$\hat{c}_1 = -10a^2\Delta^2 T_N^{-4},$$

$$\hat{c}_2 = -4a\Delta^2 T_N^{-3},$$

$$\hat{c}_3 = \Delta^2 T_N^{-2}.$$

The expansion [Eq. (7)] demonstrates that the divergence of $c|_{\max}$ is more complex than that given in Eq. (1). Indeed, in addition to the expected L^3 term, there are an infinite number of correction terms to all orders in L less than the dimensionality. The source of the corrections is just the finite lattice shift of $T_N(L)$ and is the reason why the constant

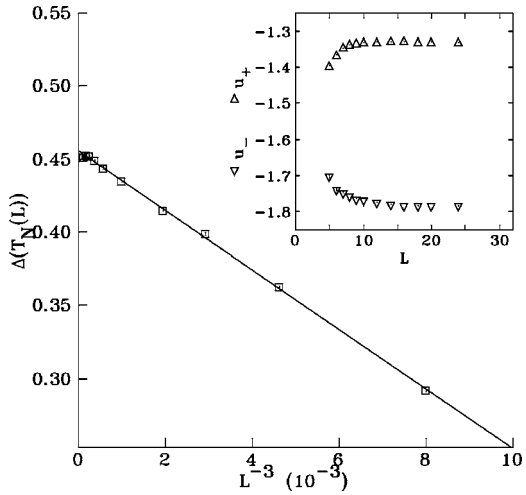

FIG. 3. Scaling of $\Delta(L)$ vs L^{-3}. For $L=\infty$ we get $\Delta_0=0.4559(6)$. In the inset we show the size dependence of u_- and u_+. For $L=\infty$ we get $u_-=-1.809\,25(15)$ and $u_+=-1.353\,35(62)$.

term c_0 in Eq. (1) would have a finite value even if the background heat capacity could be subtracted. A fit to Eq. (6) for $L>6$, with $T_N=1.7217$ and $a=0.370$ fixed (see Ref. 5), yields $\Delta=0.4574(13)$, well within the error of our less precise result $\Delta=0.455(15)$. As shown in Fig. 1(b), the fit is robust provided we omit the data for the smallest system sizes.

The last method we use to obtain the latent heat, and one that gives our most precise result, is also based on a double Gaussian $P(\epsilon)$ at $T_N(L)$. However, rather than extracting Δ from the peak height of the heat capacity/site, we extract for each system size u_+ and u_- where $c(T,L)$ is a maximum (i.e., where $w_+=w_-$). In Fig. 3 we show the difference, $\Delta(L)=u_+-u_-$ vs L^3, while in the inset we show the evolution of $u_\pm$ with increasing L. The data demonstrate that Δ contains a substantial size dependence, and the plot suggests a finite size scaling of the form

$$\Delta(L) = \Delta(\infty) + bL^{-3}. \tag{8}$$

This dependence of $\Delta(L)$ on L was not taken into account in our fit for $\Delta(\infty)$ using Eq. (6). Nor would we be able to resolve such a finite size scaling form from the divergence of $c|_{\max}$. Fitting the data to Eq. (8) for $L>6$ yields $\Delta(\infty)=0.4558(6)$ and $b=-20.0(3)$. Again, the fit is robust and agrees with the less precise results $\Delta=0.455(15)$ and $\Delta=0.4574(13)$.

Having obtained a much more precise result for the latent heat, we can now derive improved estimates of the internal energy/site and entropy/site for the disordered state at T_N. Our updated results are summarized in Table I. In the case of u_+ we achieve a 25-fold improvement, while for s_+ we achieve a 15-fold improvement.

Previously, we had calculated the latent heat using $\Delta=\sqrt{2\pi}c_3/\Gamma_3$, where the multiplicative constant $\sqrt{2\pi}$ resulted from the assumed Gaussian shape of the finite lattice heat capacity/site. Our improved estimate of Δ does not rely on any assumption regarding the shape of $c(L)$. The consistency between the estimates of Δ, however, demonstrates that the peak shape is likely to be Gaussian, which can be obscured by the temperature dependent background.

In conclusion, we have used a more precise method for obtaining the latent heat for the fcc Ising antiferromagnet. The methods developed here should be of use to others studying first order phase transitions. The increase in precision allows for better estimates of the energy and entropy of the disordered state. Furthermore, we have also shown that Δ contains significant finite size corrections which vanish to leading order as L^{-d}.

This work was supported by grants from the Natural Sciences and Engineering Research Council of Canada, and Fonds pour la formation de chercheurs et l'aide à la recherche, Québec.

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