

Thermodynamic properties of the fcc Ising antiferromagnet obtained from precision density of states calculations

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We calculate the density of states for the face-centered-cubic (fcc) Ising model with nearest-neighbor interactions using a Wang-Landau algorithm. This allows us to calculate thermodynamic quantities at all temperatures for both the ferromagnetic (FM) and antiferromagnetic (AF) models from the same data set, while avoiding the hysteresis usually occurring in models undergoing a first-order phase transition. For the FM model, our results are in agreement with high-temperature (HT) series expansion results, and are of the same precision. For the AF model which has a first-order transition, and where precise estimates of the critical behavior are lacking, we obtain $T_N=1.7217(8)$. We also obtain estimates of the free energy, internal energy, and entropy of both the ordered and disordered states at T_N with a precision comparable to that obtained in the HT series for the FM model. Details of the finite-size scaling for the AF model are discussed, and a different convergence criterion for the Wang-Landau method is introduced.

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I. INTRODUCTION

The ordering of the fcc Ising antiferromagnet has been a long-standing problem in statistical physics, dating back to the 1930s. Chemical ordering in binary alloys such as CuAu motivated the initial research, but the model is now studied primarily due to an interest in frustrated magnetism.²⁻⁴ For bipartite lattices, the solution of a ferromagnetic (FM) model immediately yields the solution of the corresponding antiferromagnetic (AF) model through a gauge symmetry. However, the fcc lattice is not bipartite. The lack of gauge symmetry serves to explain in part why, despite the existence of precision estimates of the critical behavior of the fcc Ising FM model, comparable results do not exist for the fcc Ising AF model. Here we obtain accurate estimates of basic thermodynamic quantities such as the Néel temperature (T_N), the free energy at T_N , and others with an accuracy comparable to those for the fcc Ising FM model.

The difficulty experienced with the fcc Ising AF model has two distinct sources: First, the model is geometrically frustrated resulting in an infinite ground-state degeneracy and second, the phase transition is first order. Geometrical frustration is provided by the topology of the fcc lattice where, using alloy terminology, it is impossible to assign to every Cu atom a full complement of nearest-neighbor Au neighbors and vice versa. An important consequence of geometrical frustration is that the low-temperature (LT) series expansions for the fcc Ising AF model are short^{5,6} in comparison with those of the FM model, and as such the convergence of Padé approximants to the series is poor. An additional problem is that it is not always clear which of the available ground states should be used as a starting point for the calculation⁷ of the LT series.

The first-order phase transition thought to occur in the fcc Ising AF primarily affects the accuracy obtained to date in Monte Carlo methods, since hysteresis is typically observed,^{2,3} despite the fact that the Monte Carlo method is

ergodic. The presence of hysteresis in Monte Carlo data, and elsewhere, makes the determination of a sharp phase boundary both difficult and uncertain.⁸ Furthermore, first-order transitions are not anticipated by the system approaching T_N from above (the correlation length ξ remains finite), perhaps explaining the lack of published high-temperature (HT) series.⁹

The Hamiltonian of the Ising models we consider here is

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

where the sum is over nearest-neighbor Ising spins $S = \pm 1$ on a fcc lattice with periodic boundary conditions, and $J = +1$ ($J = -1$) for the FM (AF) model, respectively. The ground states of the fcc Ising AF consist of a stack of uncorrelated, antiferromagnetically ordered, (100) planes as was first demonstrated by Luttinger.¹⁰ As there are three ways to choose the normal axis to the stacking planes, and each plane can be in one of two AF ordered states, the ground-state degeneracy is $g_0 = 3 \times 2^{2L}$ where the number of sites is $N = 4L^3$ and L is the linear dimension of the fcc lattice. It is commonly accepted^{2,3} that a first-order phase transition occurs near $k_B T_N / |J| \sim 1.76$. However, as mentioned earlier, traditional Monte Carlo methods become hampered near a first-order transition, complicating the precise estimate of T_N . Here we use a Monte Carlo method which eliminates entirely the problems caused by the first-order transition, the geometrical frustration, and the resulting large ground-state degeneracy.

II. METHODS

In a traditional Monte Carlo procedure, states are selected with a weight proportional to $g(E)\exp(-\beta E)$, with $g(E)$ being the density of states and $\beta = (k_B T)^{-1}$. Thus a new simulation is required for each value of β . New techniques such as re-weighting¹¹ have been devised to produce data at continu-

ous values of β near the simulated temperature. A completely different strategy, due to Wang and Landau,¹² is to calculate $g(E)$ directly, making it possible to calculate thermodynamic quantities at *any* temperature. For instance, the partition function Z , free-energy/site f , internal energy/site u , and heat-capacity/site c can be obtained from $g(E)$ by the standard statistical mechanics formulas:

$$Z = \sum g(E) \exp(-\beta E), \quad (2)$$

$$f = -(\beta N)^{-1} \ln(Z), \quad (3)$$

$$u = (NZ)^{-1} \sum E g(E) \exp(-\beta E), \quad (4)$$

$$c = \frac{du}{dT}. \quad (5)$$

The entropy/site s , a quantity not readily accessible using Monte Carlo (MC) methods, immediately follows from the relation $f = (u - Ts)$. We also calculate the average absolute magnetization/site, $|m(E)|$ and its square $|m(E)^2|$, for each energy level. We may then compute the average magnetization, its square, and the susceptibility from the usual formulas:

$$m = Z^{-1} \sum |m(E)| g(E) \exp(-\beta E), \quad (6)$$

$$m^2 = Z^{-1} \sum |m(E)^2| g(E) \exp(-\beta E), \quad (7)$$

$$\chi = (\beta N) [m^2 - |m|^2]. \quad (8)$$

We do not calculate the analogous AF (staggered) order parameters m_{st} , m_{st}^2 , and χ_{st} as the process is computationally expensive, and would not improve upon our estimates of T_N .

The density of states for the FM model at energy E is equal to the density of states of the AF model at energy $-E$, which allows us to obtain thermodynamic densities for both models from the *same* simulation data. This fact is especially useful since we can compare our estimates of f , u , and s at T_c for the FM model with HT series estimates, establishing the accuracy and precision of our calculated $g(E)$. Then, using this same $g(E)$, we can calculate f , u , and s at T_N for the AF model, confident that the results are of equal accuracy and precision as for the FM model.

To calculate $g(E)$ we mostly follow the prescription given by Wang and Landau,¹² and so we only give a brief description of the method here. We begin by assuming that $g(E)$ is unity, and that the initial spin configuration is random. A spin is then chosen at random and the energy before, E_i , and after, E'_i , the attempted inversion is recorded. The spin is then inverted with a probability P with

$$P(S_{i+1} \rightarrow -S_i) = \min \left[\frac{g(E_i)}{g(E'_i)}, 1 \right], \quad (9)$$

and the spin configuration is updated accordingly with the energy of the new state E_{i+1} (either E_i or E'_i) noted. Following each attempted spin inversion $g(E)$ is updated¹³ to $g(E_{i+1}) = fg(E_i)$, with the initial choice $f = \exp(1)$, and we

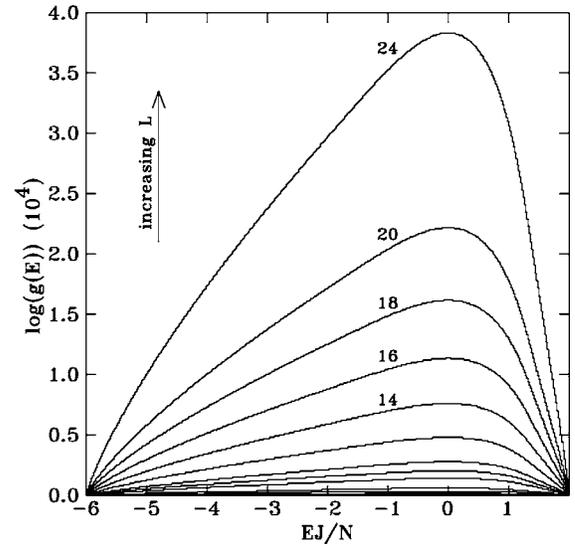


FIG. 1. Density of states $g(E)$ for the fcc Ising model for system sizes $L=2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 14, 16, 18, 20$, and 24 .

record a histogram of the number of visits to each energy state $H(E)$. If $H(E)$ is flat, then the density of states has been calculated exactly (we make more detailed comments regarding the flatness criterion near the end of this paper). However, since the original modification factor f is large, $g(E)$ is at best only approximately correct. Once $H(E)$ is determined to be reasonably flat we repeat the procedure for the n th iteration using a new f , with $f_{n+1} = \sqrt{f_n}$. Typically we use $n \sim 20$ with $10^7 - 10^8$ updates per energy level for each iteration n . Finally, the calculated $g(E)$ are normalized such that the total number of states is $\Omega = 2^N$. In Fig. 1 we have plotted the calculated¹⁴ $\ln[g(E)]$ for $2 \leq L \leq 24$. In Fig. 2 we have plotted the calculated $|m(E)|$ for the same system sizes.

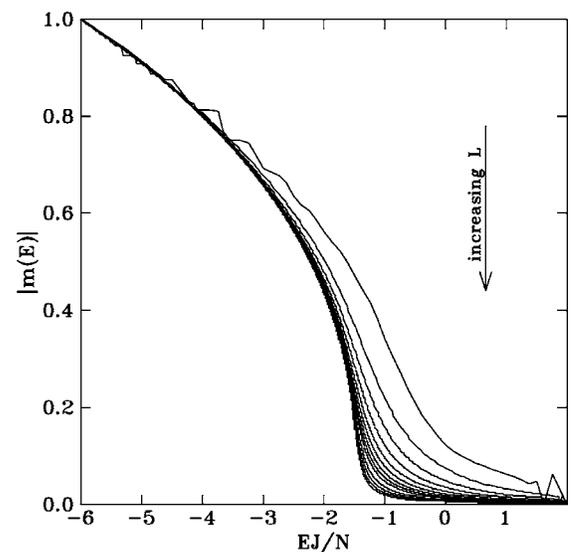


FIG. 2. Average magnetization/site at energy E , $|m(E)|$, for the fcc Ising model for system sizes $L=2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 14, 16, 18, 20$, and 24 .

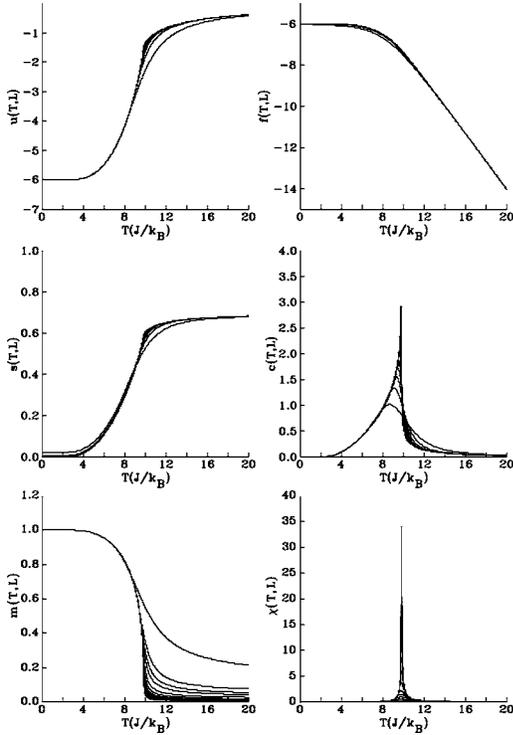


FIG. 3. Thermodynamic densities for the fcc Ising FM model, obtained from the data shown in Figs. 1 and 2.

III. RESULTS

A. Ferromagnetic model

To test the precision and accuracy of the results obtained from $g(E)$, we first compare our results for the fcc Ising FM model with those calculated from HT series expansions. In Fig. 3 we have plotted the thermodynamic densities $u(T,L)$, $f(T,L)$, $c(T,L)$, $\chi(T,L)$, $m(T,L)$, and $s(T,L)$. At T_c , one expects the free-energy/site to scale as

$$f(T_c, L) = f_0 + f_d L^{-d} \quad (10)$$

and the energy/site to scale as

$$u(T_c, L) = u_0 + u_d L^{-d+1/\nu}, \quad (11)$$

with $\nu=0.6299$, calculated from HT series for the Ising universality class.¹⁵ The scaling at $T_c=9.7943$ (T_c calculated from the HT series¹⁶) is shown in Fig. 4. A simple two-parameter fit (using $L > 4$) yields the estimates for f_0 , u_0 , and s_0 shown in Table I. Our results are in excellent agreement with the HT series estimates, having both comparable precision and accuracy. That we have been able to calculate the critical behavior of the FM fcc Ising model to better than a part in ten thousand is a testament to the high quality of our calculated density of states.

For a finite sized system, pseudotransition temperatures $T_c(L)$ can be found from the peak location of $c(T,L)$ and $\chi(T,L)$, and the maximum slope of $m(T,L)$. The pseudotransition temperatures are expected to scale according to

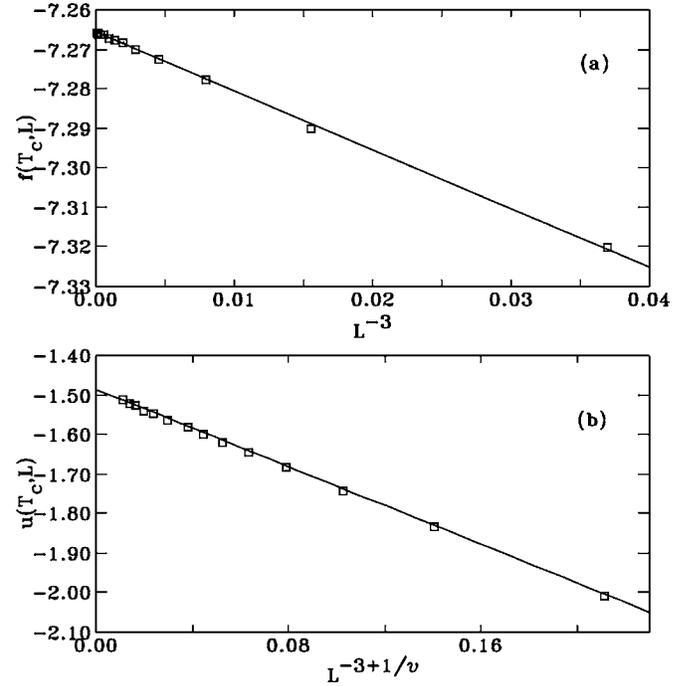


FIG. 4. Scaling of $f(T_c, L)$ and $u(T_c, L)$ at $T_c=9.7943$. Straight line fits using $L > 4$ yield $f_0 = -7.26535(3)$ and $u_0 = -1.4858(5)$ in agreement with the high-temperature series estimates $f_0 = -7.2654(3)$ and $u_0 = -1.4845(3)$.

$$T_c(L) = T_c + aL^{-1/\nu} \quad (12)$$

which allows us to locate the true transition temperature T_c . In Fig. 5 we have plotted the pseudotransition temperatures for $c(T,L)$, $\chi(T,L)$, and the maximum slope of $m(T,L)$ vs $L^{-1/\nu}$. It is clear from the plot in Fig. 5 that scaling corrections are substantial for small system sizes, and to use all of the data it would be necessary to include the scaling corrections to Eq. (12). However, by simply neglecting the data for $L < 8$, a weighted average of the three estimates of T_c yields $T_c = 9.7941(8)$, in agreement with the HT series estimate¹⁶ $T_c = 9.7943(1)$.

B. Antiferromagnetic model

While the fcc Ising FM model is well understood, the same cannot be said for the fcc Ising AF model. In the previous section we showed that our calculated $g(E)$ was ca-

TABLE I. Comparison between the results of the high-temperature (HT) series expansion and our implementation of the Wang-Landau Monte Carlo (MC) method for the fcc Ising FM model.

	HT series estimates	Wang-Landau MC
f_0	-7.2654(3)	-7.26535(3)
u_0	-1.4845(3)	-1.4858(5)
s_0	0.5902(1)	0.59009(5)
T_c	9.7943(1)	9.7941(8)

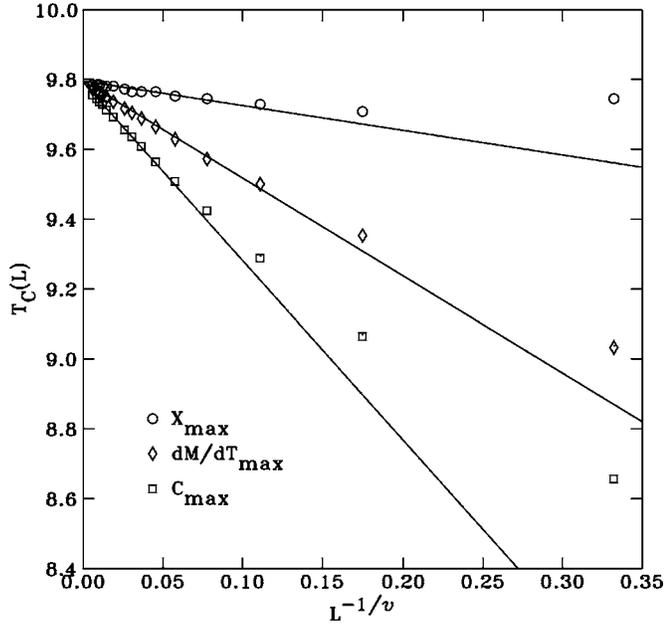


FIG. 5. Scaling of pseudotransition temperatures $T_c(L)$ for the fcc Ising FM model. Solid lines are two parameter fits to Eq. (12) using $L > 8$ (the smaller systems clearly suffer from finite-size effects). A weighted average of the three estimates yields $T_c = 9.7941(8)$, in agreement with the high-temperature series estimate $T_c = 9.7943(1)$.

pable of reproducing known results for the FM model with an error better than a part in ten thousand, comparable to the precision of HT series estimates. The exact same $g(E)$, in addition to solving the FM model, solves the AF model since $g(E)$ of the AF model is equal to $g(-E)$ for the FM model. We expect that the precision and accuracy obtained for the FM model will carry over to our analysis of the AF model, if only because the underlying data are identical. We now turn to the fcc Ising AF model where we anticipate a first-order transition near $T_N = 1.76$.

To demonstrate that the transition is first order we first show in Fig. 6 plots of the $u(T, L)$, $f(T, L)$, $c(T, L)$, $\chi(T, L)$, $m(T, L)$, and $s(T, L)$. The data indicate the presence of a first-order transition since in the approach to the thermodynamic limit (i) the energy and entropy both exhibit a discontinuity, (ii) the free energy shows a break in slope, and (iii) the heat capacity shows a delta function peak. The FM order parameters $m(T, L)$ and their fluctuations $\chi(T, L)$ are also shown, and for finite lattices they also show indications of a phase transition. However, in the thermodynamic limit the ferromagnetic order parameter vanishes.

It is often difficult to distinguish between first- and second-order transitions.⁸ A common signature for the existence of a first-order transition is the characteristic double peaked structure at T_N of $P(E) \propto g(E)\exp(-\beta E)$, the probability distribution of states with energy E . Rather than showing this feature, we simply note that the presence of a double peaked probability distribution near T_N is already apparent in Fig. 6 from the jump in the internal energy, the entropy, or even the magnetization. At $T_N(L)$, one peak in $P(E)$ represents the probability of being in a disordered metastable state

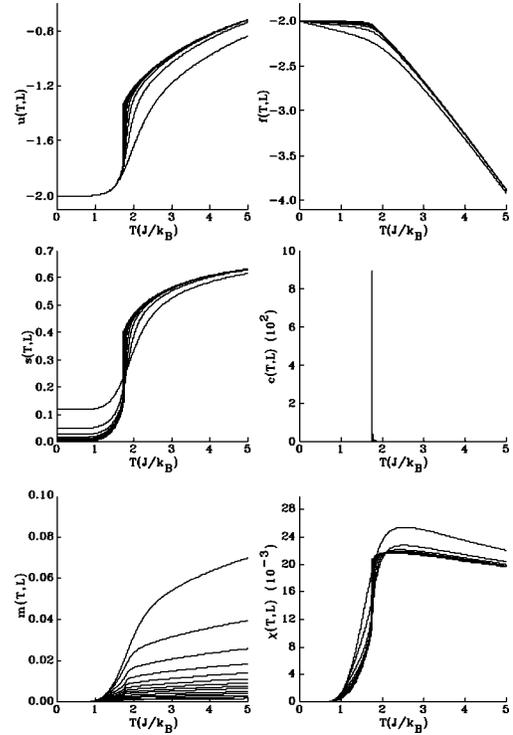


FIG. 6. Thermodynamic densities for the fcc Ising AF model, obtained from the data shown in Figs. 1 and 2.

with internal energy u_0^+ and the other peak in $P(E)$ represents the probability of being in the ordered metastable state u_0^- . Traversing $T_N(L)$, the probability associated with one state shifts to the other state, resulting in a jump in the internal energy given by the latent heat, $\Delta = u_0^+ - u_0^-$. The discontinuities, which are sharp in the thermodynamic limit, become rounded due to the finite system size as shown, for example, in Fig. 7(a) for $u(T, L)$. The rounding of the discontinuity is a good example of the problem of determining the order of a transition for a system of finite size.

The divergence of the heat capacity provides a quantitative measure of the nature of the transition. For a first-order transition, quite general arguments from the theory of thermodynamic fluctuations, or the existence of a renormalization “discontinuity” fixed point,¹⁷ implies that the heat capacity diverges as L^d . Since the divergence of the heat capacity for a second-order transition is described by the power-law relation $c \sim L^{\alpha/\nu}$, one defines for a first-order transition fictitious critical exponents $\alpha=1$ and $\nu=1/d$. The relation $\alpha=1$ follows from the expectation¹⁷ that the eigenvalue of the renormalization-group transformation, $y=1/\nu$, takes its maximal value at a first-order transition, $y=d$. In Fig. 8 we have plotted $c(T, L)$ in the vicinity of the first-order transition. The L^3 divergence of $c(T, L)$, the signal of a first-order transition, is shown in the inset (a) of Fig. 8 confirming that the transition at T_N is of first order.

To determine T_N we extract from $c(T, L)$ the pseudotransition temperature $T_N(L)$. From the earlier discussion we expect that the shift in $T_N(L)$ from $T_N(\infty)$ can be described with a fictitious critical exponent $\nu=1/d$, and thus we should have $T_N(L) \propto L^{-d}$ from Eq. (12). However, as shown in the inset

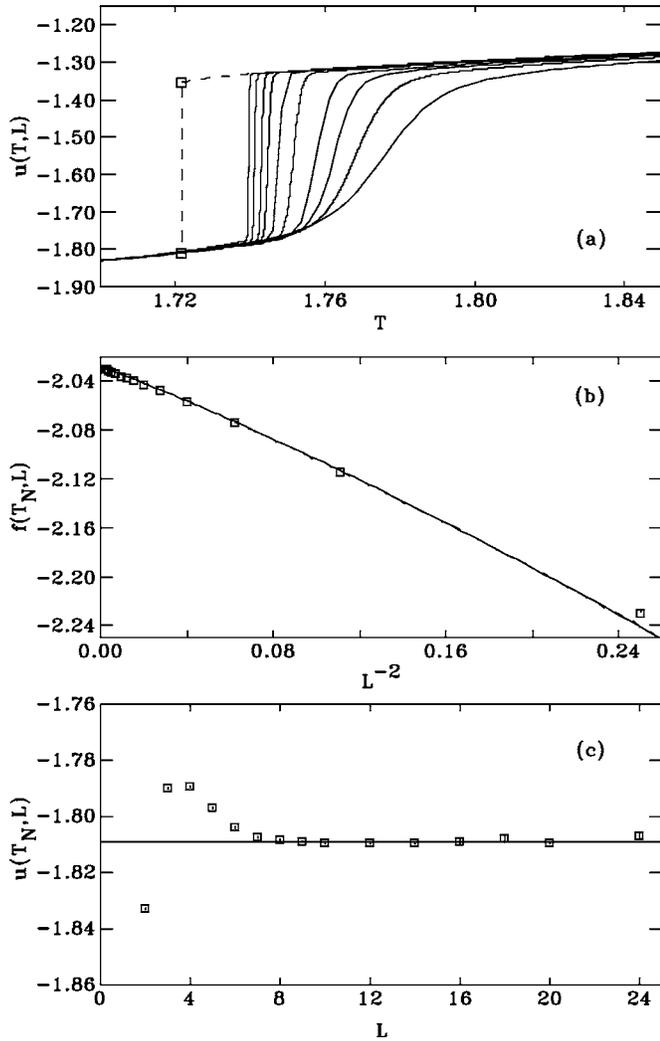


FIG. 7. In (a) we show an expanded view of the internal energy/site $u(T, L)$ in the vicinity of T_N . The dashed line shows our predicted behavior in the thermodynamic limit, with squares indicating u_0^- and u_0^+ , respectively. In (b) we show the scaling of $f(T_N, L)$ at $T_N = 1.7217$. The almost overlapping solid and dashed lines are two and three parameter fits, as discussed in the text. The fitted value, $f_2 = -0.606(9)$ is close to our anticipated result, $f_2 = -\frac{T_N}{2} \ln(2)$, validating our assignment of T_N . In (c) we show the scaling of $u(T_N, L)$. For large L , the $u(T_N, L)$ approaches a constant as expected for the first-order transition.

(b) of Fig. 8, the shift is clearly described by $T_N(L) \propto L^{-1}$ except for the smallest lattice size $L=2$. This behavior is reminiscent of the first-order transition occurring in FM Ising models with imposed boundary conditions.¹⁷ The difference between our initial expectation and our finding is a rather clear example of the difficulty associated with first-order transitions, where for example, one might incorrectly conclude that the transition is second order and $\nu \sim 1$. A two parameter fit to $T_N(L) = T_N + aL^{-1}$ using $L > 2$ yields $T_N = 1.7217(8)$. Our estimate of T_N is significantly lower than² $T_N = 1.76$.

At T_N , $f(T_N, L)$, and $u(T_N, L)$ are expected to scale according to Eqs. (10) and (11), respectively, with the relation $\nu = 1/d$. Equation (11) predicts that the internal energy should

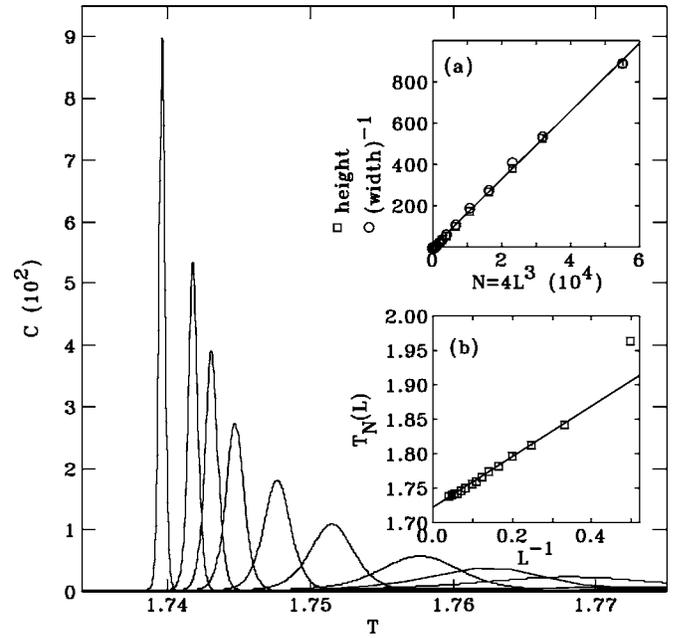


FIG. 8. $c(T, L)$ for the fcc Ising AF model in the vicinity of T_N . Inset (a) shows the L^3 divergence of the peak height and inverse half width (scaled to fit the plotting area), as expected for a first-order transition. Inset (b) shows the scaling of the pseudotransitions temperature $T_N(L)$, expected to scale as $T_N(L) = T_N + aL^{-d}$, with $d = 3$. We find instead that the data are much better described with $d = 1$, and a two-parameter fit (using $L > 2$) yields $T_N = 1.7217(8)$.

be a constant for large L . As shown in Fig. 7(c), the prediction is confirmed for $L > 7$. Note that since $T_N(L)$ approaches T_N from above, the large L behavior of $u(T_N, L)$ actually represents u_0^- , the internal energy at T_N of the metastable ordered state. A fit for $L > 7$ yields $u_0^- = -1.80925(15)$. To determine u_0^+ , we need to calculate the latent heat.

The latent heat is given by the area under the delta function peak of $c(T, \infty)$. As was shown in the inset (a) of Fig. 8, $c \sim L^d$. A two parameter fit to $c_{max}(L) = c_0 + c_d L^d$ neglecting the smallest lattice sizes yields $c_0 = 3(6)$ and $c_d = 0.0654(13)$. Since the peak height diverges as L^d , the inverse half width at half maximum, Γ , must also diverge like L^d such that the area under c is a constant, representing the latent heat. The divergence of Γ is shown in the inset (a) of Fig. 8. A two-parameter fit to $\Gamma(L) = \Gamma_0 + \Gamma_d L^d$ neglecting the smallest lattice sizes yields $\Gamma_0 = 184(86)$ and $\Gamma_d = 0.360(9)$. If we make the assumption¹⁸ that the rounded delta function is a Gaussian of height c_d and half width Γ^{-1} , then the latent heat is $\Delta = \sqrt{2\pi} c_d / \Gamma_d = 0.455(15)$. Therefore the internal energy of the metastable disordered state at T_N is $u_0^+ = -1.354(15)$. Our estimate of u_0^+ is consistent with a continuation of the high-temperature, large L , behavior of $u(T, L)$ extrapolated to T_N as shown in Fig. 7(a) where we have plotted $u(T, L)$ in the vicinity of T_N .

In the case of the free energy, Eq. (10) and the relation $\nu = 1/d$ predicts that $f(T_N, L) \sim L^{-3}$. However, as can be seen in Fig. 7(b) the data appear to scale much better using $f(T_N, L) \sim L^{-2}$. A bold, yet incorrect assertion would be that fcc Ising AF model is quasi-two dimensional. Indeed, the

TABLE II. A comparison between the results from our implementation of the Wang-Landau MC method, and those obtained by us from the low-temperature (LT) expansion coefficients of Ref. 5 using Padé approximant techniques. T_N is calculated in Ref. 18 from the data appearing in Ref. 5.

	LT series estimates	Wang-Landau MC
f_0	-2.0278(6)	-2.02809(4)
u_0^+		-1.354(15)
u_0^-	-1.814(11)	-1.80925(15)
s_0^+		0.391(6)
s_0^-	0.124(6)	0.12711(11)
T_N	1.73(0)	1.7217(8)

possibility of a reduced effective dimensionality was a motivation for the LT series expansions of Betts and Elliott.⁵

To come to an understanding of the L^{-2} scaling of $f(T_N, L)$, we write Eq. (3) as

$$f = \frac{E_0}{N} - \frac{\ln(g_0)}{(\beta N)} - (\beta N)^{-1} \left[\ln \left(1 + \sum_{k>0} g_k u^k \right) \right], \quad (13)$$

where $E_0 = -2N$ is the ground-state energy of the AF model, $u = e^{-4\beta}$ and $g_k = g(E = E_0 + 4k) / g_0$ is a polynomial in N proportional to the density of states. A further expansion of $\ln(1 + \sum_k g_k u^k)$ yields the basic starting point for the LT expansion. It is important to note that Eq. (13) is exact, and that all of the interesting information on the critical behavior is contained within the third term. For the FM model, where $g_0 = 2$, the second term of Eq. (13) is proportional to L^{-3} and together with the expected L^{-3} critical contribution of the third term, the free-energy/site can be expected to scale according to Eq. (10) with $d=3$. However, for the AF model $g_0 = 3 \times 2^{2L}$, which contributes to $f(T_N, L)$ a term $\frac{T_N}{2} \ln(2) L^{-2}$ in addition to the expected L^{-3} critical contribution of the third term. We then expect that the free energy should scale as

$$f(L) = f_0 + f_2 L^{-2} + f_3 L^{-3} \quad (14)$$

with $f_2 = -\frac{T_N}{2} \ln(2)$. A fit to Eq. (14) with $f_2 = -0.596 \dots$ fixed yields $f_0 = -2.02809(4)$, as shown in Fig. 7(b) by the solid line. Leaving f_2 as a free parameter yields only a slightly different value $f_0 = -2.02805(7)$, and $f_2 = -0.601(6)$ is still in agreement to the expected value $f_2 = -0.596 \dots$, justifying our assignment of T_N . Thus we conclude that the infinite ground-state degeneracy has the effect of masking the true value $\nu = 1/d$ expected for a first-order transition.

Unlike the FM model, where precise estimate for f_0 , u_0 and s_0 exist from the HT series, comparable results do not exist for the AF model. Nevertheless, short LT series do exist,⁵ although the estimates made from this series cannot be expected to be as precise as our Monte Carlo results. To make a comparison of our Monte Carlo results for the fcc Ising AF model we have made Padé estimates for f_0 , u_0^- , and s_0^- from the LT series expansion coefficients of Betts and Elliott, see Table II.⁵ The $[N, M]$ Padé estimates for f_0 and u_0^-

TABLE III. $[N, M]$ Padé estimates for the free energy/site taken at $T_N = 1.7217$. The free-energy series from which the Padé estimates are derived is $f = -2 - T(u^2 + 4u^3 + 15u^4 + 137/2u^5 + 8945/24u^6)$, taken from our Ref. 5. The expansion variable is $u = \exp(-4\beta)$.

	1	2	3	4	5
1		-2.027160	-2.026748	-2.027685	-2.027645
2	-2.027534	-2.026739	-2.026969	-2.027952	
3	-2.026772	-2.026980	-2.027794		
4	-2.027267	-2.028103			
5	-2.026255				

are listed in Tables III and IV. It is clear from Tables III and IV that the estimates are far from convergent. The series estimates for f_0 and u_0^- are, however, reasonable, although the scatter in u_0^- is noticeably worse.

Since the series are short and poorly convergent, we have simply calculated f_0 and u_0^- for $N+M$ a constant, and extrapolated the results to $(N+M)^{-1} = 0$. Our LT series estimate, $f_0 = -2.0278(6)$ is, somewhat surprisingly, in good agreement with our MC estimate $f_0 = -2.02809(4)$. The LT series estimate $u_0^- = -1.814(11)$ has an error two orders of magnitude larger than that for f_0 owing to the fact that the Padé estimates to u_0^- have greater fluctuations. The estimate does, however, agree with our more precise MC result $u_0^- = -1.80925(15)$. The LT series expansion estimate of T_N has previously been recalculated¹⁹ from the data appearing in Ref. 5. The estimate, $T_N = 1.73$, is near our high-precision result $T_N = 1.7217(8)$. Longer series, should they become available, would be useful in order to have a better comparison with our results.

C. Density of states

Since all of our results rely upon an accurate calculation of the density of states, it is important to check the accuracy of our calculations at this most basic level. Using the coefficients of the LT expansions it is possible to calculate $g(E)$ exactly for energies near the ground-state energy $EJ/N = -6$ of the FM model and $EJ/N = 2$ of the AF model. These exact density of states can then be compared to the approximate density of states calculated in our implementation of the Wang-Landau algorithm, which permits us to determine the

TABLE IV. $[N, M]$ Padé estimates for the internal energy/site taken at $T_N = 1.7217$. The series from which the Padé estimates are derived is $u = -2 + 8u^2 + 48u^3 + 240u^4 + 1370u^5 + 8945u^6$.

	1	2	3	4	5
1		-1.81383	-1.83484	-1.82802	-1.82177
2	-1.82969	-1.83664	-1.83024	-1.80759	
3	-1.84598	-1.83274	-1.82075		
4	-1.82662	-1.81820			
5	-1.81560				

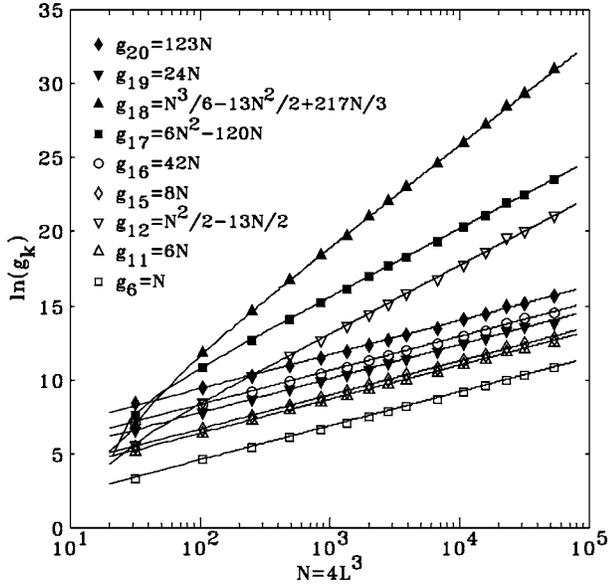


FIG. 9. Density of states divided by ground-state degeneracy, $g_k = \frac{g(E)}{g_0}$ for the fcc Ising FM model near E_0 . Points are calculated from the MC method while solid lines are g_k reconstructed from LT expansion coefficients as explained in the text.

statistical error in $g(E)$ from which all of our results are derived.

To demonstrate how this is accomplished, we expand $\ln(1+\epsilon)$ in Eq. (13) for small ϵ which yields the usual LT expansion formula:

$$f = \frac{E_0}{N} - \frac{\ln(g_0)}{(\beta N)} - \beta^{-1} \left(\sum_{k>0} b_k u^k \right). \quad (15)$$

Only those terms in g_k that are linear in N , b_k , survive the expansion, at least for the FM and AF fcc Ising models which are known to be both regular and to satisfy the Peierls condition.⁷ Using the LT series expansion coefficients b_k , for $1 \leq k' \leq k$ it is easy to calculate g_k , and therefore $g(E)$; for example $g_4 = \frac{1}{4}b_1^4 N^4 - b_1^2 b_2 N^3 + (\frac{1}{2}b_2^2 + b_1 b_3) N^2 + b_4 N$. We can therefore compare the accuracy of our implementation of the Wang-Landau method by comparing g_k calculated from the MC method to g_k calculated from LT expansions. Since we are unaware of any other method designed to check the accuracy of the Wang-Landau MC method, except for the uninteresting case where the exact solution to a particular model is already known, this test should also prove useful for other MC practitioners.

For the fcc Ising FM model, g_k are known¹⁶ to at least $k=40$. In Fig. 9 we compare the density of states measured in our implementation of the Wang-Landau MC method with those of the LT expansion for the FM fcc Ising model. In Fig. 10 the same comparison is made with the LT expansion results for the AF fcc Ising model, as calculated by Betts and Elliott⁵ up to $k=6$. Practically speaking, the two expansions (FM and AF) give us access to the regions near both end points in $g(E)$. From the comparison, we estimate that our error in $g(E)$, $\frac{\Delta g(E)}{g(E)}$, is less than 10^{-4} for the smaller lattices

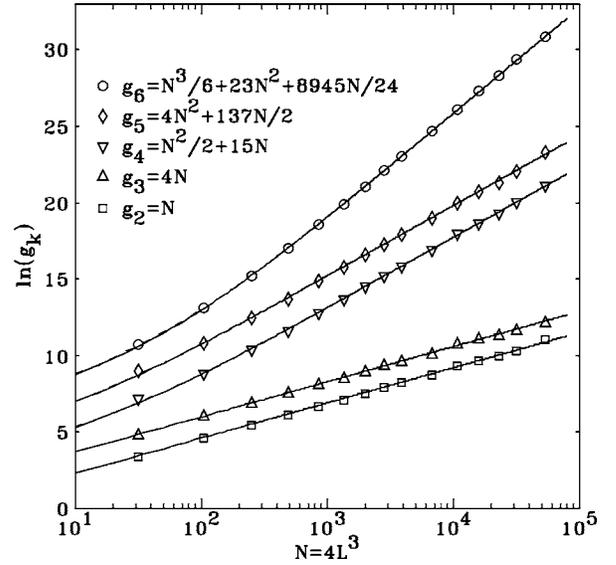


FIG. 10. Density of states divided by ground-state degeneracy, $g_k = \frac{g(E)}{g_0}$, for the fcc Ising AF model near E_0 . Points are calculated from the MC method while solid lines are g_k from LT expansion.

and less than 10^{-3} for the largest. At very small L , the MC estimate of $g(E)$ noticeably deviates from the exact calculation of $g(E)$. However, this is nothing more than an expected finite-size effect. For example, for the fcc Ising AF, finite-size effects alter the expression for g_k for $L=2$ already at $k=4$, while for $L=3$ finite-size effects do not alter the data until $k=6$.

The exact density of states can also be used as a flatness criteria when applying the Wang-Landau MC method. A typical flatness criterion is the following: When the minimal histogram entry $H_{min}(E)$ is some fixed fraction, say 99%, of the average $H(E)$ then $H(E)$ is reset to zero, f_{mod} is updated to a smaller value and the calculation of $g(E)$ proceeds. While this criterion allows the calculation to converge, it does not ensure that the calculation converges to the correct result. A superior convergence criterion would have the property that $g(E)$ be forced to converge to the exact result. However, the exact result is in our case unknown, with the exception of the small intervals around $EJ/N=-6$ (the FM ground state) and $EJ/N=2$ (the AF ground state). On the other hand, since the Wang-Landau method is based upon the idea of a random walk across the energy landscape, and the FM and AF ground states are furthest apart in energy, a test designed to ensure that these two most distant points in the random walk have the correct $g(E)$ will have the tendency to ensure that the intermediate $g(E)$ are calculated at least as well.

Based upon this idea, we have found that a better criterion is to calculate

$$\Delta^{MC} = \ln[g(E_{max})/g(E_{min})], \quad (16)$$

and compare the result to the known solution, in our case $\Delta^{EX} = \ln(3 \times 2^{2L-1})$. When $|\Delta^{MC} - \Delta^{EX}| < M$, with M some chosen convergence parameter, then $H(E)$ is reset, f_{mod} is updated as well as M , with $M * \ln(f_{mod})$ and the calculation of $g(E)$ proceeds. Typically we choose at the first iteration,

where $\ln(f_{mod})=1$, $M \sim 100$ for the smallest sizes and $M \sim 1000$ for the largest. After the first iteration, the difference between $g(E_{min})$ and $g(E_{max})$ is less than M . Following the second iteration where $\ln(f_{mod})=0.5$, the difference between $g(E_{min})$ and $g(E_{max})$ is less than $M/2$ and so on. We have found that when using this convergence test, $H(E)$ tends to a flat histogram which is a necessary condition for the successful implementation of the Wang-Landau algorithm. Indeed, our results for the FM model indicate that the $g(E)$ we have calculated is extremely accurate.

IV. CONCLUSIONS

We have employed the Wang-Landau MC method to study both the AF and FM fcc Ising models. We have also implemented a different flatness criteria which, based on our own results, indicates that the $g(E)$ converges towards the exact solution. Our results for the FM model are consistent with the HT series estimates. Our data and the HT series estimates are summarized in Table I. The same data used to calculate the properties of the FM model are then used to study the critical behavior of the AF model. We find that the

transition temperature is much lower than previously thought,² and $T_N=1.7217(8)$. Furthermore, we have found that the pseudotransition temperatures for the AF model shift from the true transition temperature as $T_N \sim L^{-1}$, similar to the shift in critical field for FM Ising models undergoing a first-order transition.¹⁷ We have also made estimates of several thermodynamic quantities at T_N , as summarized in Table II. Furthermore, we have found that at T_N , the predicted relation $1/\nu=d$ expected at a first-order transition is satisfied when scaling either the internal energy or free energy. However, in the case of the free energy we find that it is important to account for the contribution from the infinite ground-state degeneracy which would otherwise mask the true L^{-3} scaling.

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