Accurate Estimate of ν for the Three-Dimensional Ising Model from a Numerical Measurement of its Partition Function

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We give results from an accurate determination of the partition function of the three-dimensional Ising model on lattices of size up to 10^3. We compute the two complex zeros of Z closest to the real temperature axis. From a finite-size-scaling analysis of these, we get the estimates $\nu=0.6295(10)$ for the correlation-length exponent and $\phi=52.2(7)$ for the angle between the first two zeros and the real $u=e^{-4\beta}$ axis.

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We have recently developed[1-3] a new technique that directly measures the partition function of a statistical-mechanical system by numerical methods. In the present paper, we give results for some critical properties of the three-dimensional Ising model by accurately measuring its partition function on cubic lattices (with periodic boundary conditions) of size up to 10^3 using our method. The details of our numerical simulation and analysis will be published elsewhere.[4] Here we will describe our method, give results for the two zeros closest to the critical point in the $u=e^{-4\beta}$ plane and, from these, determine the correlation-length exponent ν and the angle ϕ between the first two zeros and the real $u=e^{-4\beta}$ axis.

The energy of a lattice configuration is

$$E=\frac{1}{4}\sum_{(i,j)}[1-s(i)s(j)], \quad s=\pm 1. \tag{1}$$

Here the sum is over all nearest-neighbor pairs of lattice sites. E is integer valued, ranging from zero for the ordered state to a number of the order of the volume for the maximally frustrated state. The partition function is

$$Z(u)=\sum_{E=0}^{E_m} P(E)u^E, \tag{2}$$

where $P(E)$ is the number of states of the system at energy E, $u=e^{-4\beta}$, and $E_m=dL^d/2$.

To make our simulation fast, we found it useful to update several independent lattices simultaneously. Our method to compute Z went as follows: We divided up the range of E values into sets containing four consecutive energies each. The last E value of one set was the first of the next set. Consider one of the sets. To initialize a lattice into that energy set, it was started in a disordered or ordered configuration and randomly chosen spins were flipped, the flip being accepted if the energy went in the desired direction. The independent lattices to be processed together were initialized independently.

Once all the lattices were initialized, they were updated by flipping spins at sites chosen randomly (but the same site on all the lattices in a single trial flip). If the spin flip kept a lattice within the range of allowed energy values, it was accepted. These spin-flip attempts were repeated a large number of times, and the number of times the lattice energy had a given E value was recorded. This experiment was repeated over all sets. The relative probability for the system to be in one (E) or the other (E') energy state in the set is an unbiased estimator of the relative number of states $P(E)/P(E')$ at these energy values. From the overlap in E between sets, one gets the complete partition function, apart from an irrelevant normalization factor.

The choice of four energy values in a set is to allow the system to reach any local spin configuration from any other. One could have picked more than four energies in a set. However, we believe that there are problems with ergodicity if one choses fewer than four.[5]

If one makes N independent measurements in set i, the

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TABLE I. The two zeros of the partition function closest to the infinite-volume critical point u_c as a function of lattice size L. The results shown without errors are exact (the partition function is known exactly).

	First zero		Second zero	
L	Re(u)	Im(u)	Re(u)	Im(u)
2	0.292893...	0.292893...	0	1
3	0.365053...	0.141742...	0.29311...	0.23961...
4	0.384283...	0.087739...	0.34449...	0.14330...
5	0.392787(5)	0.060978(5)	0.36579(5)	0.09833(5)
6	0.397563(5)	0.045411(5)	0.37757(5)	0.07277(5)
8	0.402718(5)	0.028596(5)	0.39011(5)	0.04535(5)
10	0.405405(5)	0.019996(5)	0.39652(5)	0.03172(5)

number N_E of times the system has energy E is distributed binomially and therefore has a known variance. The variance of $p_E = N_E/N$ is given by the binomial formula $\Delta_{p_E}^2 = N^{-1} p_E(1-p_E)$. This observation provides a method of determining the number of spin-flip attempts n_f necessary to generate an independent configuration. This can be done by increasing the number of spin-flip attempts between measurements until the measured variance settles down to the theoretical value. For all the lattices we simulated, the values of n_f for each energy were first determined in this way. Starting from the initialized lattices, for each set, we performed about $10000 n_f$ thermalizing spin-flip trials before beginning measurements. In the measuring process, successive measurements were separated by n_f steps. Note that when the energy is very small (system highly ordered), n_f is very large. This is inevitable in a local microcanonical update method such as ours. However, this is irrelevant to our results because these energy values have very little weight in the partition function as they have very little phase space, especially near $\beta = \beta_c$. Typical values we used for n_f ranged from 5 to 30.

Since the overall scale of Z is irrelevant, once the ratios $N_E/N_{E'}$ are known for all i, then defining the (arbitrary) value of $P(E_0)$ at some fixed E_0, the entire partition function is determined. The error $\Delta_{P(E)}$ in $P(E)$ can be obtained in two ways: (a) by propagating the binomial errors and (b) by repeating the measurement of the $P(E)$'s by using different values for the ratios $N_E/N_{E'}$ with Gaussian spread and computing the error from the scatter in the data. For all E values and lattice sizes we studied, these two error estimates were compatible. This is convincing evidence that not only were our measurements independent but that our errors for $P(E)$ are reliable.

We generated at least 2×10^9 independent trial flips in each set of energy values for each of the lattice sizes $L = 4$, 5, 6, 8, and 10 that we simulated. The zeros of the partition function close to the real axis were computed using a Newton-Raphson interpolation in quadrupole precision. To estimate the error in these zeros, we generated 10 estimates of Z by generating $P(E)$ values with Gaussian spread $\Delta_{P(E)}$. The standard deviation in a given zero estimated from these Z's is our error estimate for that zero.

It is known[6] that for a sufficiently large L, the zero $u_1(L)$ closest to the real positive u axis in the complex u plane obeys

$$u_1(L) = u_c + AL^{-1/\nu}[1+O(L^{-\omega})], \quad \omega > 0, \tag{3}$$

where[7] $u_c = 0.412047(10)$ is the infinite-volume critical point. Table I gives our results for the two zeros closest to the real u axis. To obtain ν, we first fit our data for $u_1(L)$ to the form

$$|u_1(L) - u_c| = a_1 L^{-1/\nu} + a_2 L^{-a_3}. \tag{4}$$

The results of this fit for $L = (2,3,4,5)$, $(3,4,5,6)$, $(4,5,6,8)$, and $(5,6,8,10)$ are shown in Table II.

Another way to get ν is to first fit the closest zero to

$$|u_1(L) - u_c| = a_1 L^{-1/\nu(L)} \tag{5}$$

for successive values of L and then use the $\nu(L)$ values to fit to

$$\nu(L) = \nu + a_4 L^{-a_5}. \tag{6}$$

The $\nu(L)$ and ν values from fits to Eqs. (5) and (6)

TABLE II. Results for the estimate of ϕ and ν. The fits shown alongside $L = 2,3,4,5$ in column 5 are for lattice sizes $L = (2,3,4,5)$, $(3,4,5,6)$, $(4,5,6,8)$, and $(5,6,8,10)$, respectively. The fits shown alongside $L = 2,3,4,5$ in column 4 are for lattice sizes (2,3,4,5,6,8,10), (3,4,5,6,8,10), (4,5,6,8,10), and (5,6,8,10), respectively.

		ν		
L	ϕ	From Eq. (5)	From Eq. (6)	From Eq. (4)
2	67.5		0.62924(35)	0.630(1)
3	53.7...	0.54055...	0.62841(52)	0.629(2)
4	54.4...	0.59429...	0.6282(10)	0.629(3)
5	54.2(1)	0.61300(14)	0.6285(20)	0.628(2)
6	53.8(1)	0.62043(30)		
8	53.0(1)	0.62492(28)		
10	52.8(2)	0.62684(52)		

are also given in Table II. We use two successive L values to estimate $\nu(L)$ from Eq. (5) and then use the $\nu(L)$ values to estimate ν from Eq. (6).

This last fit was made by two methods: (a) a least-squares fit using a simplex method, and (b) keeping a_5 fixed, and making a linear fit to a constant plus $a_4 L^{-a_5}$. a_5 was then varied to obtain a maximum value for the regression coefficient. Both methods agree perfectly. The errors were computed as the scatter in the fits generated by using 100 initial data with Gaussian spread. The fits to Eq. (6) were repeated by removing successively the $L=2$ data, $L=3$, etc., always obtaining a consistent value for ν (although the errors increase). When making this fit of column 3 of Table II to Eq. (6), it is not clear what L values to use for the entries in column 3 because the data there were obtained from two successive L values (L,L'). A compromise (which probably represents the best choice) is to use $(L+L')/2$ (and this is the fit shown in column 4 of Table II) which gives $\nu=0.629\,24(35)$. Using instead L one gets $\nu=0.631\,15(42)$ and using L' one gets $\nu=0.628\,07(36)$. The average of these three values is $\nu=0.629\,49$. From the fact that all the fits represented in columns 4 and 5 of Table II agree within errors, we conclude that we are already in the regime of lattice sizes values that extrapolates smoothly to $L=\infty$, as far as estimates of ν are concerned. We should therefore be able to estimate ν reliably. From similar considerations, we decided that our data were not accurate enough to estimate ω [Eq. (3)]. In principle, the second zero should also scale with L as $L^{-1/\nu}$. Although the ν values obtained this way are consistent with those from the first zero, they are not accurate enough to be competitive.

Our final estimate of ν is 0.6295(10), where the central value is defined as the average of the values obtained when fitting Eq. (6) with different interpretations of L as explained before, and to be conservative we have multiplied by three the actual error of this fit. This is also meant to account for the smallness of the L values used in the analysis and the possible occurrence of correlation in the data.

We have also analyzed our data using the extrapolation techniques discussed by Barber.[8] In particular, extrapolating the $\nu(L)$ values in column 3 of Table II by the alternated ϵ algorithm gives $\nu=0.6299$ in perfect agreement with the value obtained above.

In Ref. 6 it was shown that as $L\to\infty$, the angle ϕ that the tangent to the line of zeros at u_c makes with the real u axis is related to the specific-heat exponent α, and the ratio A_+/A_- of the specific-heat singularity amplitude above (small β) and below (large β) the critical temperature. However, it has recently been shown that the formula derived in Ref. 6 is valid only for the high-index zeros.[9] We are unable to measure high-index zeros with accuracy sufficient to use the results of Ref. 6 (for details of how we decide the error on the zeros, see Ref. 1). However, we can measure the angle (which we shall also call ϕ), between the first two zeros and the real u axis. These angles for various lattice sizes are also given in Table II. One could estimate the thermodynamic limit of these angles by extrapolating the data to $L\to\infty$. Using a linear fit of the last four numbers in column 2 of Table II and extrapolating to $L=\infty$ gives the estimate $\hat{\phi}=51.5°$. However, strictly speaking, the extrapolation function is unknown and the errors on our angles are big. We therefore estimate ϕ as the average of our angle $\phi(10)$ for $L=10$ and the value $\hat{\phi}$. This gives $\phi=52.2(7)$ degrees. The error we estimate to be $0.5[\phi(10)-\hat{\phi}]$. Our result for ϕ is quite different from that of an earlier study by Marinari.[10] However, the accuracy of the measurement of ϕ in Ref. 10 was a factor of about 50 poorer than ours.

Using the relationship between α and A_+/A_- from Ref. 6 and assuming the validity of hyperscaling, one would get $A_+/A_-=0.31(6)$. This also disagrees with the experimental value (0.36 to 0.63) for this ratio for the reason stated above that the formula in Ref. 6 is valid only for large-index zeros.

The behavior of Z near the antiferromagnetic transition is obtained already from the zeros in Table I. Indeed, it is easy to see that in arbitrary dimensions, on lattices of size L^d with L even and with periodic boundary conditions, $P(E)=P(E_m-E)$. This gives [see Eq. (2)]

$$Z(u)=u^{E_m}Z(u^{-1}). \tag{7}$$

Hence, the line of zeros representing the antiferromagnetic phase transition is obtained from those for the ferromagnetic by the replacement $u\to u^{-1}$. This also shows that the value of ν in the two cases is the same. Another way of seeing this is to note that for any configuration at positive β with total action $S=\sum_{i,\mu}s_i s_{i+\mu}$, there is another with action $-S$ which has the same weight in the partition function of the antiferromagnet (at $-\beta$). This antiferromagnetic configuration is obtained in any dimension from the ferromagnetic configuration by making a checkerboard pattern (even-odd sites) and by the change of variables $s\to -s$ on the even or odd sites.

We are very encouraged to have managed to compute ν to an accuracy comparable to the best series expansion and extrapolation techniques.[11] We are currently extending our analysis to larger lattices to measure correlations and the magnetic susceptibility from which we hope to extract other exponents. The partition functions we have computed are available on request.

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