Low-Temperature Expansion for the Ising Model

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On simple cubic lattices, we compute the low-temperature expansion for the energy of the Ising model through 50 excited bonds in three dimensions and 44 excited bonds in four dimensions. We also give the magnetization through 42 excited bonds. Our method is a recursive enumeration of states with given energies on a set of finite lattices with generalized helical boundary conditions. A linear combination of such lattices cancels finite volume effects.

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High- and low-temperature expansions are a major technique for the study of critical properties of statistical systems and field theories. These series usually involve a diagrammatic analysis which becomes rapidly more complex as the order increases. Thus it would be interesting to have an automated technique for the generation of the relevant terms.

Here we consider the low-temperature expansion for discrete systems. Our approach does not involve explicit graphs, but relies on a recursive computer enumeration of configurations. We illustrate the approach on the three-dimensional Ising model.

Series expansion results have not thus far been competitive with numerical simulations [1]. We believe our method gives them the potential to do so. Our methods are similar in spirit to those of Ref. [2], the primary difference being our use of generalized helical lattices.

For the Ising model, the low-temperature series amounts to an enumeration of low-energy excitations. We find the infinite volume series for the energy through 50 excited bonds, substantially extending the previous result [3] of 36, an order comparable to existing high-temperature expansions [4].

The method relies on a procedure due to Binder [5] for the exact solution of discrete models on small lattices. In Ref. [6] these ideas were further developed. The present paper adds further tricks to Ref. [7], which explored using these exact solutions to extract the low-temperature series.

We consider the Ising model on a simple cubic lattice. On each site i is a spin σ_i taking the values ± 1. The system energy is

$$E=\sum_{\{i,j\}}(1-\sigma_i\sigma_j)-H\sum_i\sigma_i\,, \tag{1}$$

where the first sum is over nearest neighbors of spins, each pair being counted once. Temporarily we set the applied field H to zero. The partition function is the sum of the Boltzmann weight over all configurations

$$Z=\sum_{\{\sigma\}}e^{-\beta E}\,. \tag{2}$$

We define $P(E)$ to be the number of states with a given energy E. Thus, we have

$$Z=\sum_{E=0}^{6N}P(E)u^{E/2}\,, \tag{3}$$

where N is the number of sites and $u=e^{-2\beta}$.

We compute the coefficients $P(E)$ exactly on small systems. We recursively assemble the system one site at a time. The starting point is a list of all states and corresponding energies for a single transverse layer of the lattice. All spins outside this layer are frozen to the same value; that is, the boundary conditions in the longitudinal direction are cold. Spins are then sequentially freed to build up the lattice in this third direction. We store the exact number of states of any given energy and specified exposed top layer. Storing the top layer in the bits of an integer I, we define $p(E,I)$ to be this count. When a new spin or set of spins is added, we obtain the new counts $p'(E,I)$ as a sum over the old counts,

$$p'(E,I)=\sum_{I'}p[E-\Delta(I,I'),I']\,. \tag{4}$$

Here I' can differ from I only in the bits representing the newly covered spins, and $\Delta(I,I')$ is the change in energy from any newly changed bonds. For the present analysis we add the spins one at a time. Thus, the sum in the above equation is only over the two possible values for the newly covered spin. After the lattice is grown, a sum over the top layers gives the resulting $P(E)=\sum_I p(E,I)$.

As the temperature goes to zero, so does the variable u. Thus Eq. (3) is the low-temperature expansion for Z. From it, we compute the series for the average energy, $\langle E\rangle=2(u\,\partial/\partial u)\ln(Z)$. Comparing this expectation before and after adding the last spin, we obtain the average energy per new site. Expanding in powers of u gives

$$\langle E/N\rangle=\sum_j e_j u^j\,. \tag{5}$$

We are interested in the coefficients e_j in the infinite volume limit. Table I gives the values of these coefficients through $j=50$ for the three-dimensional and through order $j=44$ for the four-dimensional Ising models. Note that any enclosed group of flipped spins always involves an even number of excited bonds; thus, the ex-

TABLE I. The low-temperature expansion coefficients for the average energy per unit volume for the three- and four-dimensional Ising model on a simple cubic lattice.

i	e_i (3D)	e_i (4D)
0	0	0
2	0	0
4	0	0
6	12	0
8	0	16
10	60	0
12	−84	0
14	420	112
16	−1056	−144
18	3756	0
20	−11 220	1120
22	37 356	−2816
24	−118 164	2032
26	389 220	11 856
28	−1 261 932	−46 704
30	4 163 592	66 960
32	−13 680 288	94 576
34	45 339 000	−707 472
36	−150 244 860	1 545 120
38	500 333 916	−148 656
40	−1 668 189 060	−9 522 864
42	5 579 763 432	30 130 576
44	−18 692 075 820	−30 299 808
46	62 762 602 860	
48	−211 062 133 044	
50	711 052 107 060	

pansion only contains even powers of u.

Reference [7] showed a version of helical boundaries whereby an $n\times n$ transverse slice is mimicked with only $(n^2+1)/2$ sites. Here we extend this idea to include the helicity into the longitudinal direction.

We build our lattices one site at a time; so, it is natural to imagine the sites lying in a line. We do not, however, consider sequential sites as nearest neighbors. Instead, we introduce three integer parameters (h_x,h_y,h_z) representing the distance along the line to the nearest neighbor in the corresponding x, y, or z direction. Labeling sites in the sequence by their ordinal number i, the nearest neighbors of site i are at $i\pm h_x$, $i\pm h_y$, and $i\pm h_z$. For convenience, assume $h_x<h_y<h_z$. With this convention, all sites more than h_z steps back in the chain are covered. Thus the recursion only requires us to keep explicit track of the h_z "exposed" spins at the end of our chain.

A minimal closed loop consists of a number of steps such that $n_xh_x+n_yh_y+n_zh_z=0$, where n_i represents the number of steps in the ith direction. On an infinite cubic lattice the only solution is the trivial case $n_i=0$. On a finite lattice, any other solution represents a finite-size correction. One way to visualize our lattice is to consider an infinite lattice, and identify all points lying in a plane orthogonal to **h**.

Flipping a chain of n spins along a minimal closed path generates a state with $4n$ excited bonds, and creates a potential error in the series at that order. For example, $(h_x,h_y,h_z)=(19,21,24)$ with $(n_x,n_y,n_z)=(3,-5,2)$ gives a minimal loop of length 10. This system will correctly give the series to the same order as a 10^3 lattice.

Given parameters (h_x,h_y,h_z), it is straightforward to enumerate the minimal closed paths. The contribution to the coefficients e_i from a particular path is independent of any permutations or sign changes in the numbers (n_x,n_y,n_z). This allows us to combine results from various size lattices to cancel the contributions from particular closed loops. For example, consider loops of length 9. The (16,18,21) lattice has a minimal such loop with steps $\mathbf{n}=(3,2,-4)$, the (16,17,21) lattice has closed loops with steps (1,4,−4) and (5,−1,−3), the (13,18,20) lattice has closed loops with (2,3,−4) and (4,−4,1), and finally the (14,17,19) system has the loops (3,2,−4) and (5,−3,−1). If we combine the coefficients e_i as obtained from these lattices with weights (2,1,−1,−1), respectively, then all errors from the loops of length 9 cancel out.

This procedure extends to cancel further loops. In addition to these simple closed loops, there are double loops which involve a set of flipped spins wrapping around the lattice simultaneously in two directions. We rejected double loops of energy less than or equal to the order to which we were working.

We assembled a list of 20 lattices with relative weights to cancel all loops of length less than 13. These systems involved values of h_z through 22. A closed loop of 13 flipped spins has 52 excited bonds. This is the limit of the order of the series presented here.

We must store counts for all energies up to the max-

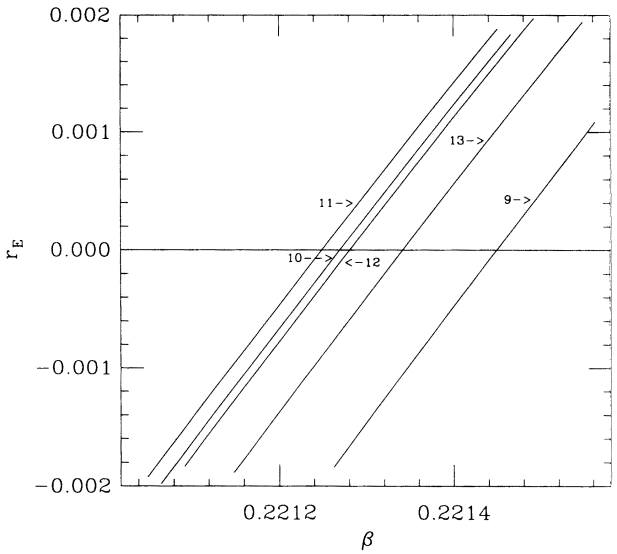

FIG. 1. The ratio r_E defined in Eq. (6) in the vicinity of the Ising critical point. The series expansion for this quantity was Padé approximated in $z=3u^2/(1+3u^2)$ as the ratio of two polynomials, and the curves are labeled by the highest power of z appearing in the numerator.

imum order desired, as well as for all possible values of the top h_z spins of our helical lattice. Thus, the primary computational problem is storage. To reduce these demands, we performed the calculations modulo small integers so that at intermediate stages the counts could be stored in one byte each. This gives the final coefficients modulo the given integers. The entire program is then repeated multiple times using different values for the modulos. The Chinese remainder theorem states that if you know a number modulo a set of mutually prime numbers, then it is uniquely determined up to the product of these numbers. We made sufficient passes to make this product larger than the desired coefficients, and then extracted them with a short search procedure.

From our results we constructed the series for the ratio

$$r_E = \frac{(u\,\partial/\partial u)E}{(u\,\partial/\partial u)^2 E}. \tag{6}$$

As the first three e_i vanish, this ratio is determined through order u^{42}. At the critical point r_E should have a zero. The slope at this zero equals $2/\alpha$, where α is the specific heat exponent.

A ratio test shows that the first singularity for the series is unphysical and occurs near $u^2 = -\frac{1}{3}$. We therefore made a conformal transform to new variables defined by $z = 3u^2/(1+3u^2)$ to map the interval $u^2 = [-\frac{1}{3}, 0]$ to $z = [-\infty, 0]$ and the physical interval $u^2 = [0, \infty]$ to $z = [0, 1]$. We then did a Padé analysis in the variable z. The results of these are shown in Fig. 1 where we plot a few stable Padé series for r_E in the vicinity of the expected singularity in β. Our estimate for the critical point is $\beta_c = 0.22132(7)$ and for the exponent is $\alpha = 0.207(4)$. The error quoted is just from averaging over the five Padé series in Fig. 1, and is rather dependent on details of the analysis. Although the location of the critical point is in

TABLE II. Coefficients c_{ij} for the expansion of the magnetization. Here $\frac{1}{2}\langle 1-\sigma\rangle = \sum_{i,j} c_{ij} u^i \lambda^j$, where $u = e^{-2\beta}$ and $\lambda = e^{-2\beta H}$. Unlisted coefficients for $i \leq 42$ all vanish.

i	$j=1$	2	3	4	5
6	1	0	0	0	0
8	0	0	0	0	0
10	0	6	0	0	0
12	0	−7	0	0	0
14	0	0	45	0	0
16	0	0	−108	12	0
18	0	0	64	332	0
20	0	0	0	−1314	240
i	$j=4$	5	6	7	8
22	1620	2130	108	0	0
24	−651	−14020	2976	56	8
26	0	27660	9450	2646	0
28	0	−23040	−132867	27216	2448
30	0	7031	387444	−9520	36976
32	0	0	−508428	−1101660	179172
34	0	0	320220	4722564	−848904
36	0	0	−78904	−8833328	−7580660
38	0	0	0	8680245	51142152
40	0	0	0	−4397652	−130897242
42	0	0	0	909434	180175480
i	$j=9$	10	11	12	13
28	216	0	0	0	0
30	1143	240	0	0	0
32	49896	3960	264	36	0
34	360450	41310	7260	0	0
36	547236	672670	73216	12960	1248
38	−12320586	2368080	773025	138744	9516
40	−35804700	−6147840	6632208	1220220	311688
42	492777576	−124127630	4660084	9776508	2129660
i	$j=14$	15	16	17	18
36	0	0	0	0	0
38	1596	0	0	0	0
40	32760	2520	240	0	0
42	379400	62700	1920	408	54

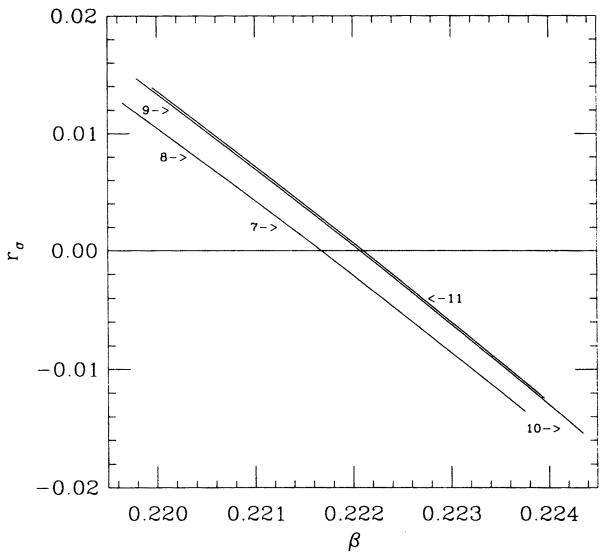

FIG. 2. The same as Fig. 1, but now for the ratio r_σ in Eq. (8).

excellent agreement with Monte Carlo estimates [1], we found that it was somewhat sensitive to the order of the series. On the other hand, α is about twice the expected value. The small value for this quantity makes its accurate determination difficult.

Extending these results to include the magnetic term in Eq. (1), we augmented the counting to keep track of the number of flipped spins as well as excited bonds. This increases memory demands, so we reduced the highest energy to 42 excited bonds, and worked on a combination of smaller lattices with h_z up to 17 to cancel closed loops of length through 10. Assuming a spin-up background, we write

$$\tfrac{1}{2}\langle 1-\sigma\rangle=\sum_{i,j} c_{ij} u^i \lambda^j, \tag{7}$$

where $\lambda=\exp(-2\beta H)$. The coefficients c_{ij} through 42 excited bonds are given in Table II.

Summing the numbers in Table II over rows gives the expansion in u^2 for the magnetization at zero applied field. In Fig. 2 we show several Padé approximants for the ratio

$$r_\sigma=\frac{\langle\sigma\rangle}{u\,\partial\langle\sigma\rangle/\partial u} \tag{8}$$

in the vicinity of the critical point. Before making these approximants, we made the same change of variables as used for Fig. 1. These give an estimate for $\beta_c=0.22192(2)$ and the exponent $\hat{\beta}=0.308(5)$, where $\hat{\beta}$ is defined by $\langle\sigma\rangle\propto(\beta-\beta_c)^{\hat{\beta}}$ in the critical region. These numbers are also in good agreement with the accepted values.

The set of parameters defining the helical lattice increases in higher dimensions, giving more lattices for combination tricks. Also, a cluster with a given number of spins in more dimensions tends to have a larger number of excited bonds. In preliminary studies of the four-dimensional model we used a combination of 4 lattices with transverse volume up to 21, from which we extract the series for the energy through 44 excited bonds. These coefficients are also given in Table I.

These methods should easily generalize to other discrete systems. The helical lattices used, as well as the combinations to cancel out finite-size errors, are independent of the Ising nature of the spins. It is straightforward to introduce additional couplings, although this will increase memory needs. Some interesting possibilities for further exploration are gauge, Potts, and coupled gauge-spin models in various dimensions. Changing boundary conditions should enable the study of interface properties. A direct application of these counting methods to the high-temperature or strong-coupling limit may also be quite useful. In Ref. [8] similar recursive methods were suggested as a means to study many fermion systems. A particularly challenging problem is the extension of these ideas to theories with continuous spins.

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