Low temperature expansion for the 3-d Ising Model

by

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ABSTRACT

We compute the weak coupling expansion for the energy of the three dimensional Ising model through 48 excited bonds. We also compute the magnetization through 40 excited bonds. This was achieved via a recursive enumeration of states of fixed energy on a set of finite lattices. We use a linear combination of lattices with a generalization of helical boundary conditions to eliminate finite volume effects.
Expansions about either infinite or vanishing coupling 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 generating the low temperature or weak coupling 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.

The method uses a procedure of Binder [1] for the explicit solution of discrete models on small lattices. In Ref. [2] these ideas were further developed. Ref. [3] explored extracting the low temperature series. This paper adds further tricks to obtain additional terms. This extends the low temperature series to an order comparable to existing high temperature expansions [4].

We consider the Ising model on a three dimensional simple cubic lattice. On each site $i$ is a spin $\sigma_i$ taking the values $\pm 1$. The system energy is

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

where the first sum is over all nearest neighbor pairs 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

$$Z = \sum_{\langle \sigma \rangle} e^{-\beta E}$$

Sorting configurations by energy, we rewrite this as a sum over $E$. We define $P(E)$ to be the number of states with a given energy $E$. Thus, we have

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

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

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We compute the coefficients $P(E)$ exactly on small systems. We recursively assemble the system one site at a time. The method enables us to build up a lattice with arbitrary length in one of the three dimensions. Intermediate stages require an explicit enumeration of all exposed two dimensional slices. This effectively reduces the computational complexity to that of a system of one less dimension.

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

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

(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 two terms, representing the two possible values for the newly covered spin. After the lattice is grown, a sum over the top layers gives the resulting $P(E) = \sum_I p(E, I)$ We always continue the recursion sufficiently to avoid finite size errors in the longitudinal direction.

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 per site, $\langle E \rangle = 2 \left( u \frac{\partial}{\partial u} \right) \log(Z)$. Comparing this expectation before and after adding the last spin, we obtain the average energy per new site. Expanding in powers of $u$ gives

$$\langle E/N \rangle = \sum_j e_j u^j$$

(5)

We are interested in the coefficients $e_j$ in the infinite volume limit. One of our primary results, given in Table I, is the values of these coefficients through $j = 48$.

At zero temperature ($\beta = \infty$) the only surviving states have all spins parallel. As the temperature increases, groups of spins can flip in this uniform background. Enumerating
the possible combinations gives a diagrammatic method to obtain the low temperature coefficients [5]. Note that any enclosed group of flipped spins always involves an even number of excited bonds. Thus the expansion only contains even powers of \( u \). We use a combination of periodic transverse and cold longitudinal boundary conditions to ensure this remains true on our finite systems.

On a periodic lattice of size \( n \times n \times n \), the order to which the weak coupling expansion for \( \langle E/N \rangle \) will agree with the infinite volume limit is \( 4n - 2 \). A line of \( n \) flipped spins can wrap around the lattice and have energy \( 4n \) rather than the \( 4n + 2 \) it would have in infinite space. This order can be increased via boundary conditions to require more spins to be flipped to wrap around the lattice. Ref. [3] showed a version of helical boundaries whereby an \( n \) by \( n \) 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 on such a lattice consists of a number of steps such that \( n_x h_x + n_y h_y + n_z h_z = 0 \), where \( n_i \) represents the number of steps in the \( i \)th direction. The length of such a loop is \( n = |n_x| + |n_y| + |n_z| \). On an infinite cubic lattice the only solution to these equations is the trivial case \( n_i = 0 \). On a finite lattice, any other solution represents a finite size correction. Flipping a chain of spins along such a closed path generates a state with \( 4n \) excited bonds, and creates a potential error in the series at that order. For a simple 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 and will 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. A different set of \( h_i \) corresponds to a different set of such paths. However, the
contribution to the coefficients $e_i$ from a particular path is, by symmetry, 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 $n = (3, 2, -4)$, the $(16, 17, 21)$ lattice has closed loops with steps $(1, 4, -4)$ and $(5, -1, -3)$, the $(13, 18, 20)$ lattice has a 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 gives the series to the same order as a lattice with the smallest loop having length 10, which otherwise requires at least 24 sites.

This procedure extends to cancel further loops. For our calculation, we assembled two lists of 10 lattices and the relative weights for combining them to cancel all loops of length less than 13. We ran both combinations as a check on the error cancellations. The first set involved lattices with $h_z$ up to 23, and took about a day on an IBM RS6000 workstation. The second set, involving up to $h_z = 24$, used about half a day on a 32K Connection Machine and about a day of Cray-YMP time.

Each lattice used had a minimal loop of length at least 9. While a loop of length 13 has 52 excited bonds, we have a potential error at order 50 because of the possibility of a more complex loop wrapping around the lattice simultaneously in a length 9 and a length 10 direction. The minimal energy of such a possibility is 50 excited bonds. This is the limit on the order of the series presented here.

During the recursive construction, each new count is a trivial sum of just two terms, representing the two possibilities for the covered spin. On the other hand, we must store counts for all energies up to the maximum 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 substantially 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. After multiple passes using mutually prime values for these modulos, we use the Chinese remainder theorem to reconstruct the final series.
From our results we constructed the series for the ratio

\[ r_E = \frac{(u \frac{\partial}{\partial u})E}{(u \frac{\partial}{\partial u})^2 E} \]  

(6)

As the first three \( e_i \) vanish, this ratio is determined through order \( u^{42} \). \( r_E \) should have a zero at the critical point, with the slope at this zero equal to \( 2/\alpha \) where \( \alpha \) is the specific heat exponent.

The ratio test showed that the first singularity for the \( E \) series is unphysical and occurs near \( u^2 = -1/3 \). We therefore made a conformal transform to new variables defined by \( z = 3u^2/(1 + 3u^2) \) to map the interval \( u^2 = [-1/3, 0] \) to \( z = [-\infty, 0] \) and the physical interval \( u^2 = [0, \infty] \) to \( z = [0, 1] \). We then did a Pade analysis in the variable \( z \). The results of these are shown in Fig. 1 where we plot a few stable Pade series for \( r_E \) in the vicinity of the expected singularity in \( \beta \). There is a clear zero near \( \beta = 0.22 \), in good agreement with the Monte Carlo studies [6] which give \( \beta_c = 0.22165 \). The average slope of the various curves in Fig. 1 gives \( \alpha = 0.22 \), which is about twice the accepted value for this exponent. 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 20 excited bonds, and worked on a combination of smaller lattices with \( h_z \) up to 19 to cancel closed loops of length 8 through 10. Assuming a spin up background, we write

\[ \frac{1}{2}(1 - \sigma) = \sum_{i,j} c_{ij} u^{2i} \lambda^j \]  

(7)

where \( \lambda = \exp(-2\beta H) \). The coefficients \( c_{ij} \) through 20 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 Pade approximants for the ratio

\[ r_\sigma = \frac{\langle \sigma \rangle}{u \frac{\partial \langle \sigma \rangle}{\partial u}} \]  

(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 \( \beta_c = 0.222 \) and the
exponent $\hat{\beta} = 0.31$, where $\hat{\beta}$ is defined by $\langle \sigma \rangle \propto (\beta - \beta_c)^{\hat{\beta}}$ in the critical region. These numbers are in reasonable agreement with the accepted values.

The method presented here 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. [7] 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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Figure Captions

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 Pade 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.

Fig. 2. The same as Fig. 1 but now for the ratio $r_\sigma$ in Eq. (8).
| $i$ | $e_i$          |
|-----|---------------|
| 0   | 0             |
| 2   | 0             |
| 4   | 0             |
| 6   | 12            |
| 8   | 0             |
| 10  | 60            |
| 12  | -84           |
| 14  | 420           |
| 16  | -1,056        |
| 18  | 3,756         |
| 20  | -11,220       |
| 22  | 37,356        |
| 24  | -118,164      |
| 26  | 389,220       |
| 28  | -1,261,932    |
| 30  | 4,163,592     |
| 32  | -13,680,288   |
| 34  | 45,339,000    |
| 36  | -150,244,860  |
| 38  | 500,333,916   |
| 40  | -1,668,189,060|
| 42  | 5,579,763,432 |
| 44  | -18,692,075,820|
| 46  | 62,762,602,860|
| 48  | -211,062,133,044|
Table II. Coefficients $c_{ij}$ for the expansion of the magnetization. Here $\frac{1}{2}\langle 1 - \sigma \rangle = \sum_{i,j} c_{ij} u^{2i} \lambda^j$ where $u = e^{-2\beta}$ and $\lambda = e^{-2\beta H}$. Unlisted coefficients for $i \leq 20$ all vanish.

| $i$ | $j = 1$ | 2 | 3 | 4 | 5 |
|-----|---------|---|---|---|---|
| 3   | 1       | 0 | 0 | 0 | 0 |
| 4   | 0       | 0 | 0 | 0 | 0 |
| 5   | 0       | 6 | 0 | 0 | 0 |
| 6   | 0       | -7| 0 | 0 | 0 |
| 7   | 0       | 0 | 45| 0 | 0 |
| 8   | 0       | 0 | -108| 12| 0 |
| 9   | 0       | 0 | 64| 332| 0 |
| 10  | 0       | 0 | 0 | -1,314| 240|

| $i$ | $j = 4$ | 5 | 6 | 7 | 8 |
|-----|---------|---|---|---|---|
| 11  | 1,620   | 2,130| 108| 0 | 0 |
| 12  | -651    | -14,020| 2,976| 56| 8 |
| 13  | 0       | 27,660| 9,450| 2,646| 0 |
| 14  | 0       | -23,040| -132,867| 27,216| 2,448|
| 15  | 0       | 7,031| 387,444| -9,520| 36,976|
| 16  | 0       | 0 | -508,428| -1,101,660| 179,172|
| 17  | 0       | 0 | 320,220| 4,722,564| -848,904|
| 18  | 0       | 0 | -78,904| -8,833,328| -7,580,660|
| 19  | 0       | 0 | 8,680,245| 51,142,152|
| 20  | 0       | 0 | 0 | -4,397,652| -130,897,242|

| $i$ | $j = 9$ | 10 | 11 | 12 |
|-----|---------|----|----|----|
| 14  | 216     | 0  | 0  | 0  |
| 15  | 1,143   | 240| 0  | 0  |
| 16  | 49,896  | 3,960| 264| 36 |
| 17  | 360,450 | 41,310| 7,260| 0 |
| 18  | 547,236 | 672,670| 73,216| 12,960|
| 19  | -12,320,586| 2,368,080| 773,025| 138,744|
| 20  | -35,804,700| -6,147,840| 6,632,208| 1,220,220|

| $i$ | $j = 13$ | 14 | 15 | 16 |
|-----|---------|----|----|----|
| 18  | 1,248   | 0  | 0  | 0  |
| 19  | 9,516   | 1,596| 0  | 0  |
| 20  | 311,688 | 32,760| 2,520| 240|