Series expansions without diagrams

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ABSTRACT

We discuss the use of recursive enumeration schemes to obtain low and high temperature series expansions for discrete statistical systems. Using linear combinations of generalized helical lattices, the method is competitive with diagramatic approaches and is easily generalizable. We illustrate the approach using the Ising model and generate low temperature series in up to five dimensions and high temperature series in three dimensions. The method is general and can be applied to any discrete model. We describe how it would work for Potts models.

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Introduction

Expansions about either infinite or vanishing coupling have long been a major technique for the study 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 a fully automated technique for the generation of the relevant terms.

Here we discuss a purely mechanical method to generate the low and high temperature expansions for discrete systems. The approach does not involve explicit graphs, but rather relies on a recursive computer enumeration of configurations. We illustrate the approach on Potts and Ising models, although it is considerably more general.

The method is based on a recursive transfer matrix procedure of Binder [1] for the explicit solution of discrete models on small lattices. Enting [2] discussed how to combine such solutions on small lattices to obtain low temperature series. Guttmann and Enting have pushed this finite lattice method to obtain rather high order low temperature series for the three dimensional Ising model [3]. Our approach is similar in spirit to this work, although it differs in many technical details. In Ref. [4] these ideas were further developed in the context of finite size scaling and the analytic structure of the partition function. Ref. [5] explored using these exact counting procedures on helical lattices to extract the low temperature series. Helical lattices have been further generalized in Ref. [6] enabling one to calculate the low temperature series for the three dimensional Ising model to 50 excited bonds. Ref. [7] applied these methods to Potts models in two and three dimensions.

This paper is primarily intended to explain these methods in more detail and explore extensions. In a recent preprint Vohwinkle [8] has adapted the diagrammatic shadow method to obtain Ising and Potts expansions to several more terms than we have been able to obtain. Our method is, however, quite general and easy to implement. It is an open question whether some of the ideas of Ref. [8] can be adapted into our scheme to get even longer series.

Recursive counting

We begin with a discussion of the recursive approach to solving small systems exactly.
This section will also serve to establish notational conventions. We illustrate the basic method with the Ising model on a finite three dimensional simple cubic lattice. On each site $i$ is a spin $\sigma_i$ taking the values $\pm 1$. The energy of the system is

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

(1)

where the sum is over all nearest neighbor pairs of spins, each pair being counted once. At inverse temperature $\beta$, the partition function is the sum of the Boltzmann weight over all configurations

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

(2)

Organizing the set of configurations by their energy, we rewrite this as a sum over $E$. This introduces the density of states function $P(E)$ representing the number of states of the system with the given energy $E$. Thus, we have

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

(3)

where $N$ is the number of sites and $u = e^{-2\beta}$. If we consider, for example, an $N^3$ lattice, there will be $2^{N^3}$ states, but the solution for the partition function can be expressed in terms of $\mathcal{O}(N^3)$ integers $P(E)$.

For a given lattice we compute the coefficients $P(E)$ exactly using a transfer matrix to assemble the system one site at a time. This recursive construction enables us to build up a lattice with arbitrary length in one of the three dimensions. For the series analysis it is important to always continue the recursion sufficiently to avoid finite size errors in this “longitudinal” direction. At intermediate times the process requires an explicit enumeration of any exposed two dimensional slice. This effectively reduces the computational complexity to that of a system of one less dimension. Thus the solution of an $N^3$ lattice requires, at most, the explicit enumeration of only $2^{N^2}$ states. This enables us to work with sizes which would be impractical for an explicit enumeration of all states.

The starting point of the method 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. At intermediate stages the computer stores the exact number of states of any given energy and specified exposed top layer. Storing the top layer as the bits of an integer $I$, 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 $I'$ runs over all integers differing from $I$ at most in the bits representing the newly covered spins, and $\Delta(I, I')$ is the change in energy from any newly changed bonds. In Ref. [5] the spins were added one layer at a time, while here we add them one at a time. Thus for the present calculation 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 $P(E)$ for the entire system

$$P(E) = \sum_I p(E, I).$$

(5)

The low temperature series

Note that as the temperature goes to zero so does the variable $u$. Thus Eq. (3) is itself the low temperature expansion for $Z$. From it, we compute the corresponding series for the average energy per site,

$$\langle E \rangle = \frac{\sum_E E P(E)}{Z} = 2 \left( u \frac{\partial}{\partial u} \right) \log(Z)$$

(6)

Comparing this expectation value before and after the last spin is added, we obtain the increase in the average energy per new site. Expanding this in powers of $u$ gives

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

(7)

We are interested in the coefficients $e_j$ in the infinite volume limit.

At zero temperature ($\beta = \infty$) the only states which survive have all spins parallel. As the temperature increases, groups of spins can flip in this uniform background. A single
flipped spin has 6 excited bonds, and thus $e_6$ represents the first non-trivial term in our expansion. In our units, each excited bond has energy 2 and there are 6 such bonds for a single flipped spin; thus we have $e_6 = 12$. Continuing to more complicated combinations of flipped spins gives the usual diagrammatic method to obtain the further coefficients.

Note that any enclosed group of flipped spins must always have an even number of excited bonds. Thus the expansion only involves even powers of $u$. Our method of construction is such that when a spin is added to the helix, we account for the energy of both the forward and backward bonds at once. This, combined with the cold boundary conditions at both ends, ensures that we generate only even powers of $u$ in our expansions.

**Helical lattices**

Computing $Z$ exactly 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 $4N - 2$. At this order a line of $N$ flipped spins can wrap around the lattice and show finite size effects. Such a configuration will have energy $4N$ rather than the $4N + 2$ it would have in infinite space. This is the smallest excitation affected by boundary effects and hence, on a periodic lattice of size $N$, the expansion is valid through $O(4N - 2)$.

The order to which the series is correct can be increased by changing the boundary conditions to require more spins to be flipped to wrap around the lattice. Ref. [5] showed how a version of helical boundaries allowed an $N \times N$ transverse slice to be mimicked with only $[(N^2 + 1)/2]$ sites. Here we extend this idea to include the helicity into the direction in which the lattice is grown.

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, we assume

$$h_x < h_y < h_z \quad (8)$$

With this convention, as we grow our lattice, all sites more than $h_z$ steps back in the chain
are covered. Thus the recursive methods of Refs. (1-3) only require us to keep explicit track of the $h_z$ “exposed” spins at the end of our chain. The computational work grows exponentially with this number; thus, we wish to keep $h_z$ as small as possible.

A minimal closed loop on such a lattice consists of a number of steps in each spatial direction such that

$$n_x h_x + n_y h_y + n_z h_z = 0.$$  \hspace{1cm} (9)

Here $n_i$ represents the number of steps in the $i$–th direction. The length $n$ of such a loop is

$$n = |n_x| + |n_y| + |n_z|$$  \hspace{1cm} (10)

$n$ is the “effective” periodic size of the lattice for our series construction, and, as argued above, the series is correct to $O(u^{4n-2})$. On an infinite cubic lattice the only solution to Eq. (9) 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. As a simple example, $(h_x, h_y, h_z) = (3, 4, 5)$ with $(n_x, n_y, n_z) = (1, -2, 1)$ gives a minimal loop of length 4. Such a lattice will give the series equivalent to that on a $4^3$ lattice, but with only $h_z = 5$ sites in cross section. Similarly, $(h_x, h_y, h_z) = (19, 21, 24)$ has closed loops of length 10 corresponding to $(n_x, n_y, n_z) = (3, -5, 2)$. Here 24 sites mimic a 10 by 10 cross sectional lattice, thus saving a factor of $2^{76}$ in computational effort.

Note that Eq. (9) tells us that if we regard $n$ and $h$ as vectors, they are orthogonal. Thus a simple way to visualize our lattice is as an infinite one with all sites which lie in any single plane orthogonal to $h$ as identified with each other. Fig. (1) attempts to show this construction. Considering the plane through the origin, all the sites lying in this plane themselves form a lattice. Closed loops that contribute finite size corrections consist of sets of flipped spins connecting the sites of this lattice.

** Cancelling loops **

We now discuss how forming linear combinations of the energy series coefficients from a set of finite helical lattices can give the infinite volume series to a higher order than any
individual lattice in the set. The approach here differs in details but is similar in essence to the combining of partition functions in the finite lattice method of Refs. [2] and [3].

Given a set of parameters \((h_x, h_y, h_z)\), it is straightforward to enumerate the minimal closed paths. A different set of parameters corresponds to a different set of such paths. However, any erroneous contribution to the coefficients \(e_i\) from a particular such path is, by symmetry, independent of any permutation or sign changes in the numbers \((n_x, n_y, n_z)\). This allows us to push the series further, by combining the results on various size lattices to cancel the contributions from particular closed loops.

For an explicit 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 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 would require at least 24 sites.

This procedure extends to cancel further loops. It is straightforward to write a program to enumerate the closed loops on various lattices, and then solve the linear equations to cancel the errors from such loops. In Table I we present a list of 26 lattices and the relative weights for combining them to cancel all loops of length less than 14. Note that in this way we have reduced what would naively require a \(14^3\) lattice to a set of calculations involving a cross section of at most 24 spins.

After cancelling the single loops as above, a potential problem arises from more complicated diagrams which wrap around the lattice simultaneously in two or more ways. This would correspond to flipping a set of spins which connects three of the identified sites in Fig. (1). In selecting our lattices for Table I we did not consider any system which had a loop contributing to any order for which we were extracting the series coefficient.

It is easy to calculate the order at which these more complex loops contribute. In our lattice finding program we first find the three closest identified sites which do not lie on a single straight line. (Double loops connecting points in a line are automatically cancelled
at the same time as the simple loops.) Denote the minimum distances between these three images as $d_1$, $d_2$, and $d_3$. In most cases, the minimal way of flipping a set of spins to wrap around these three loops produces an energy of $(d - 1) \times (d_1 + d_2 + d_3 - 2) - 2$, where $d$ is the dimension of the system. We rejected using any lattices for which this number is at or below the order to which we were extracting the series.

In rare special cases this formula needs a correction. The energy can be lower if one of the fundamental loops has no steps in one direction. Then the two loop diagram can run into its periodic image, reducing the relevant order. For example, with the $h = (11, 15, 18)$ lattice, the fundamental loops have $n = (0, 6, -5), (3, -1, -1)$ and $(3, 5, -6)$. The minimal energy for a set of flipped spins which connects these three images is 52 bonds, rather than the predicted 54 from the above formula. Needless to say, this lattice caused us considerable consternation.

The utility of these cancellations depends strongly on dimension. For two dimensions with at most $h_y$ sites on the top row, the best solution is always a single lattice with $h_x = h_y - 1$. In this case the shortest extraneous loop has $n = (h_y, -h_y + 1)$ with length $2h_y - 1$. Note that as $h_y$ becomes large, the transfer matrix effectively grows the lattice along a diagonal.

For higher dimensions, on the other hand, there are a rapidly growing number of interesting lattices to cancel loops between, and this method becomes particularly powerful. Table II includes a list of 15 lattices which give the four dimensional series through order 50 excited bonds. Although the largest lattice here has 28 sites in the top row, the tricks of the next section are also more effective in four dimensions, so this is not a particularly difficult case.

Note that although we have been discussing these lattices in the context of the Ising model, the results are more general. In particular, the combinations in Table I are valid for any nearest neighbor model on a simple cubic lattice.

These methods can also be applied to other than simple cubic lattices. For example, to treat a body centered cubic lattice, each site has eight neighbors, so we need four components for $h$. We can merely use a four dimensional lattice-finding program modified to require the real closed loops of length 3 be present and not be cancelled.
Table I. A combination of 26 lattices which gives the three dimensional low temperature expansion coefficients through 54 excited bonds. The first column represents the coefficient with which the lattice is to be weighted and the second gives the vector $\mathbf{h}$ which defines the lattice.

| Coefficient | $(h_x, h_y, h_z)$ |
|-------------|------------------|
| 1           | (17,23,24)       |
| 2           | (19,22,24)       |
| -1          | (19,21,24)       |
| 3           | (19,20,23)       |
| -1          | (18,20,23)       |
| -4          | (11,15,23)       |
| -1          | (18,21,22)       |
| 3           | (16,21,22)       |
| -2          | (18,19,22)       |
| -3          | (15,19,22)       |
| 3           | (14,19,22)       |
| -3          | (16,17,22)       |
| -3          | (5,18,21)        |
| 3           | (8,17,21)        |
| 3           | (7,19,20)        |
| -6          | (1,17,20)        |
| 6           | (16,18,19)       |
| -2          | (16,17,19)       |
| 6           | (12,17,19)       |
| 7           | (8,17,18)        |
| -3          | (7,16,18)        |
| -9          | (11,14,18)       |
| -7          | (8,13,18)        |
| 2           | (9,16,17)        |
| 3           | (1,13,15)        |
| 4           | (12,13,14)       |

**Miscellaneous tricks**

During the recursive buildup of the lattice, each new count is the sum of just two terms, representing the two possibilities for the covered spin. Thus the arithmetic involved is rather trivial. On the other hand, we must store counts for all energies up to the maximum order desired as well as for all relevant values of the top $h_z$ spins of our helical lattice. In addition, the intermediate counts can become rather large numbers. Thus, the
Table II. A combination of 15 lattices which gives the four dimensional low temperature expansion coefficients through 50 excited bonds. The first column represents the coefficient with which the lattice is to be weighted and the second gives the vector $\mathbf{h}$ which defines the lattice.

| Coefficient | $(h_x, h_y, h_z)$ |
|-------------|------------------|
| 3           | (15,24,25,28)    |
| -27         | (15,21,25,28)    |
| 14          | (13,20,25,28)    |
| 27          | (15,20,26,27)    |
| 16          | (11,20,26,27)    |
| 18          | (19,20,25,27)    |
| 2           | (11,15,25,27)    |
| -4          | (16,17,23,27)    |
| -13         | (14,17,19,27)    |
| -6          | (11,20,25,26)    |
| -4          | (15,18,25,26)    |
| -16         | (15,21,23,26)    |
| -16         | (7,20,24,25)     |
| 28          | (14,15,23,25)    |
| -21         | (17,18,22,25)    |

primary computational problem is storage. To substantially reduce these demands, we calculated the series coefficients several times, each time modulo a small different integer. Depending on the integers chosen, this enabled us at intermediate stages to store the counts in either one byte or one short integer each. As all operations are simple additions or multiplications, this procedure correctly 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. This theorem states that if you know a number modulo a set of relatively prime integers, then the number is uniquely determined up to the product of those integers.

As we are repeating the series calculations for several different modulos and for several different lattices and only combining the results at the end, this problem is particularly suitable for trivial parallelization. Indeed, except for the most memory intensive cases, we have experimented quite successfully with sending different lattice-modulo combinations to a farm of workstations. For this we have been using the Condor distributed batch system.
Note that as we add spins, the energy of the system can only increase. This means that we never need counts involving more excited bonds than the order to which we are evaluating the series. Furthermore, while the recursive procedure is predicated on keeping all top rows for the lattice, this is not actually necessary if we only want the series to some given order. In particular, we need not store any counts for top rows which already contain more excited bonds than the order we are working to. To handle this, we use a simple subroutine that, given a possible top row, finds the next top row in numerical sequence with a number of excited bonds less than or equal to the working order.

As an explicit example with the Ising model, consider the $h = (17, 23, 24)$ lattice and allowing only up to 54 excited bonds. In this case we need keep only 2,778,176 of the possible $2^{24} = 16,777,216$ possible top rows. In four dimensions, because there are additional bonds which can be excited, the corresponding reductions are even larger.

In addition to not keeping all top rows, we need not store counts with less energy than the minimum possible for a given top row. That is, while for the top row with all spins up we need to keep counts for all possible excitation energies up to the order under consideration, if the top row has a single flipped spin we need only keep counts of at least 3 excited bond pairs, and so on. Finally, for the Ising case on a simple cubic lattice with our boundary conditions there can only be an even number of excited bonds. In this way, the above $(17, 23, 24)$ lattice requires keeping track of 11,259,428 individual $p_0(E, I)$, or less than one count per possible top row.

During the recursion, each new count is the sum of one or two of the old ones, corresponding to whether the covered spin is flipped or not, and whether for a flipped spin we do not already have more energy than being considered for the count in question. A simple way to implement this is to have two index arrays, with the elements of each representing the location of the old counts to be used. Having an entry in the index array out of bounds provides a simple way to flag those cases where only a single term goes into the sum. Once the geometry is established by the construction of these arrays, the program simply loops over the counts, making the new values the sum of two old ones pointed to by these indices. In this way all the complications of setting up the geometry need only be done once per
One can save additional memory by not storing the full indices, but using the fact that if one orders the counts first by top row numerically, and then by bonds, the respective indices always change by relatively small numbers in going from one count to the next. Thus we need only store the changes rather than the indices themselves. In the main loop the new indices are obtained by a simple addition to the previous ones. The index changes for our studies could all be stored in a single byte.

A final trick that we have so far only used minimally is to invert a partially grown lattice on itself. The idea is that given the counts for all possible top layers, we can then obtain the counts for a lattice roughly twice as long with all possible specified layers in the middle. Calling this count \( p_d(E, I) \), we have

\[
p_d(E, I) = \sum_{E_1, E_2} p(E_1, I)p(E_2, I_r)\delta(E, E_1 + E_2 - d(I))
\] (11)

where \( I_r \) has the bits of \( I \) in reversed order (because the lattice has been flipped upside down) and \( d(I) \) represents the excited bonds inside the middle layer. The latter is removed to prevent double counting. This technique can provide information on correlation functions in this middle layer. As all states are known explicitly, any such correlation function can be obtained exactly with no significant additional drains on computer time or memory. As a simple example, this provides an alternative method for obtaining the magnetization series to that discussed in the next section.

Other observables

So far we have been discussing the direct low temperature expansion for the partition function or, equivalently, the average energy or the specific heat. The method easily extends to other observables by generalizing the counts. For example, consider applying a magnetic field by generalizing the partition function to

\[
Z = \sum_{\{\sigma\}} e^{-\beta E - H \sum_i \sigma_i}
\] (12)

Derivatives with respect to the applied field give us a procedure to compute the magnetization

\[
M = \langle \sigma_i \rangle = -\frac{1}{N} \frac{\partial}{\partial H} \log Z
\] (13)
and the magnetic susceptibility

\[ \chi = \frac{\partial}{\partial H} M \]  \hspace{1cm} (14)

For general \( H \) one can expand observables simultaneously in \( u \) and \( \lambda = e^{-2H} \). In Ref. [6] this possibility was discussed in terms of generalizing the counts \( P(E) \) to the two indexed count \( P(E, S) \), representing the number of states of a given bond energy and number of flipped spins \( S \). The recursion relations for these counts are completely analogous to those for \( P(E) \). The double series for the magnetization was presented up to order 42 excited bonds in Ref. [6].

One difficulty with this approach is the increased memory required for storing counts for all magnetizations as well as energies. If one is only interested in the magnetic properties in the zero field limit, one can store considerably less. In particular, consider moments of the magnetization, from which quantities such as the susceptibility are easily extracted. It is convenient to define new quantities

\[ P_k(E) = \sum_S S^k P(E, S). \]  \hspace{1cm} (15)

With this definition, \( P_0(E) \) is simply the original count \( P(E) \). The zero field magnetization is easily found from

\[ M = 1 - 2 \sum E P_1(E) e^{-\beta E} \frac{1}{NZ}. \]  \hspace{1cm} (16)

Finally, from \( P_2 \) we can obtain the magnetic susceptibility

\[ \chi = 4 \left( \frac{\sum E (P_2(E) - P_1(E)^2) e^{-\beta E}}{NZ} \right). \]  \hspace{1cm} (17)

The advantage of working with these moments is that they themselves satisfy simple recursion relations. To derive them, consider the generalization of Eq. (4)

\[ p'(E, S, I) = \sum_{I'} p(E - \Delta(I, I'), S - \Delta_s(I'), I'). \]  \hspace{1cm} (18)

Here \( p(E, S, I) \) is the number of states of energy \( E \), with \( S \) flipped spins, and with lattice top row specified by \( I \), and \( p' \) is the same quantity on the new lattice obtained after adding the new spin. We denote by \( \Delta_s(I') \) the change in the number of flipped spins; that is, \( \Delta_s = 1 \) if the new spin is flipped (the relevant bit of \( I' = 1 \)) and \( \Delta_s = 0 \) otherwise.
Now define the moments,

\[ p_k(E, I) = \sum_S S^k p(E, S, I). \]  

(19)

Taking moments of Eq. (18) now gives the recursion relations for the \( p_k \)

\[ p'_0(E, I) = \sum_{I'} p_0(E - \Delta, I') \]  

\[ p'_1(E, I) = \sum_{I'} p_1(E - \Delta, I') + \Delta_s(I)p_0(E - \Delta, I') \]  

\[ p'_2(E, I) = \sum_{I'} p_2(E - \Delta, I') + 2\Delta_s(I)p_1(E - \Delta, I') + \Delta_s^2(I)p_0(E - \Delta, I'). \]  

(20) (21) (22)

The first of these relations is just our original recursion, and the others enable us to calculate the magnetization and susceptibility with the addition of only two new counts.

It is straightforward to derive the analogous counting schemes for n-point susceptibilities and their various spatial moments, like the second moment of 2-point susceptibility \( \mu_2 = \langle x^2 \sigma_x \sigma_0 \rangle \). In later cases however there are some conceptual difficulties connected to the ambiguity of the definition of the coordinate on the helical lattice. Some more work needs to be devoted to this problem.

**Strong coupling**

We now turn to the application of the counting methods to the strong coupling series. In this section we describe the procedure for the three dimensional Ising model, although again it is easily generalized. As before we consider spins \( S_i \) on the lattice sites \( i \) and taking the values \( \pm 1 \). The partition function of Eq.(2) can be trivially rewritten

\[ Z = \left( \frac{1 + e^{-2\beta}}{2} \right)^{N_i} \sum_\sigma \prod_{\{i,j\}} (1 + \sigma_i \sigma_j \tanh(\beta)) \]  

(23)

where the product is over all lattice links and \( N_l \) is the number of links in the system. For the strong coupling series we consider small \( \beta \) and expand the above sum in powers of \( \tanh(\beta) \). Each term involves a set of selected bonds which each give a power of \( \tanh(\beta) \). Having selected a set of bonds, we can then perform the sum over the spins. If any site
has an odd number of selected bonds emanating from it, the sum will vanish. Otherwise
the sum over any given spin gives a factor of two. Thus we conclude

\[ Z = 2^N \left( \frac{1 + e^{-2\beta}}{2} \right) N \sum_k N(k) (\tanh(\beta))^k \]  

(24)

Here \( N(k) \) represents the number of possible ways to select \( k \) bonds in such a manner that
each site is the end of an even number of selected bonds. We adapt our counting methods
to evaluate these numbers \( N(k) \).

As before we maintain information on the top layer of our lattice while adding new
sites one at a time. Here, however, rather than the values of the spins themselves on the
top layer, we keep information on the selected bonds ending there. In particular, because
we want to allow future bonds to extend above the top row, we relax the constraint that
an even number of bonds end on the top sites. Thus, we keep a count \( N(k, I) \) where \( I \)
now stores in its set bits those sites with an odd number of bonds coming into them from
previous sites. We refer to sites with an odd number of incoming bonds coming into them from
previous sites. We refer to sites with an odd number of incoming bonds as having “loose
ends” or “dangling bonds.” On adding a new site, we have the basic recursion relation

\[ N'(k, I) = \sum_{I'} N(k - \Delta(I, I'), I') \]  

(25)

where \( \Delta(I, I') \) represents the number of selected bonds attached to the new spin and \( I' \) is
related to \( I \) via changes in those bits representing sites attached to the new one.

In three dimensions, for any given \((k, I)\) there will be four terms in the above sum
over \( I' \). This represents a factor of two for whether the new \( x \) bond is selected times a
factor of two for whether the new \( y \) bond is chosen. Whether the corresponding \( z \) bond is
chosen or not is determined by the corresponding bit of \( I \) which determines if an even or
odd number of bonds are selected.

An immediate factor of two in memory is saved because each bond has two ends. This
means that if no bonds enter from outside below the lattice, the top layer must have an
even number of loose ends. Any top layers with an odd number of loose ends need never be
kept. In practice, instead of looping over all given any integers \( I \) representing the dangling
bonds from an allowed configuration, we need only loop over the right \( h_z - 1 \) bits of \( I \) and
can determine the allowed leftmost bit by parity considerations.
We work with generalized helical lattices as before. For simplicity in initialization, we set all counts to zero except for $I = 0$, representing no dangling bonds. This may seem a bit peculiar because we do not allow loops to enter and travel through the bottom layer. It is, however, simple to implement and boundary conditions in the longitudinal direction are irrelevant if we grow the lattice long enough.

On a single helical lattice, the strong coupling series will be correct to the order of the first chain of bonds which wraps around one of the artificial closed loops discussed earlier. The double loop criterion is somewhat different now; here it is only the total length of a loop which wraps around two directions that matters. Rejecting lattices with such double loops, we can perform the same cancellation between lattices as in the low temperature series.

The strong coupling series can be extended significantly by using the fact that all valid loops of links on an infinite lattice will have an even number of selected bonds in any of the coordinate directions. We use this fact by calculating the counts several times, but including extra minus signs when adding bonds in various directions. For example, if we first find the series giving every $x$ bond a weight of -1, we can then add the result without this extra sign and any artificial diagram involving an odd number of $x$ bonds will cancel out. Thus we need not worry about any finite size effects involving an odd number of steps in the $x$ direction. Repeating the procedure 8 times for all combinations of minus signs for the three possible directions, we can ignore any extraneous closed loops with an odd length along any dimension. Similarly, any double loops with an odd number of steps in any direction can also be ignored. Without this trick the order to which the strong coupling series can be found is rather uninteresting.

With these tricks, we have found the series through 20 selected bonds from the combination of lattices given in Table (III). As the lattice size goes to infinity, we write the free energy in the form

$$F = \frac{\log(Z)}{N_S} = \log 2 + \frac{N_L}{N_S} \log \left( \frac{1 + e^{-2\beta}}{2} \right) + \sum_k f_k (\tanh(\beta))^k$$

(26)

where $N_S$ and $N_L$ denote the number of sites and links, respectively. To extract the
Table III. A combination of 11 lattices which gives the three dimensional strong coupling series through order 20. The first column represents the coefficient with which the lattice is to be weighted and the second gives the vector $\mathbf{h}$ which defines the lattice.

| coefficient | $(h_x, h_y, h_z)$ |
|-------------|-------------------|
| 4           | (4,15,16)         |
| 2           | (12,13,16)        |
| -4          | (4,13,16)         |
| -6          | (11,12,16)        |
| 4           | (7,12,16)         |
| 6           | (11,14,15)        |
| -4          | (7,13,15)         |
| 3           | (5,11,15)         |
| 3           | (9,13,14)         |
| -3          | (4,12,13)         |
| -3          | (8,11,13)         |

Table IV. The coefficients for the strong coupling series for the three dimensional Ising model through order 20. The $f_k$ are defined in the text.

| k  | $k f_k$ |
|----|---------|
| 0  | 0       |
| 2  | 0       |
| 4  | 12      |
| 6  | 132     |
| 8  | 1,500   |
| 10 | 19,800  |
| 12 | 288,528 |
| 14 | 4,468,380 |
| 16 | 72,236,124 |
| 18 | 1,206,062,448 |
| 20 | 20,649,134,532 |

coefficients $f_k$, it is somewhat easier to work with the analog of an expectation,

$$
\langle k \rangle = \sum_k \frac{k N(k)}{\sum_k N(k)} \rightarrow N \sum_k k f_k
$$

(27)

As for the low temperature series, we extract the contribution per spin by comparing the counts before and after adding the last spin. Since they are just combinations of integer
counts, the products $k f_k$ themselves are always integers, while the $f_k$ are not in general. We tabulated these numbers through order 20 in Table (IV). These numbers are not new; for example they plus one additional term follow from the results in Ref. [3].

**Potts models**

As we mentioned earlier, the application of the counting techniques to the low temperature series expansions is very easily generalizable to any discrete system with nearest neighbor interaction. To illustrate this, consider the $q$-state Potts model, defined by the interaction of the form

$$E = \sum_{\langle ij \rangle} [1 - \delta_{\sigma_i,\sigma_j}]$$

(28)

where $\sigma_i$ is a site-defined field that takes $q$ possible values. The sum is taken over all nearest neighbor pairs of spins with $\delta$ being the Kronecker symbol.

Writing the partition function in the form

$$Z = \sum_{E=0}^{dN} P(E)u^E$$

(29)

with $d$ being the spatial dimension and $u = e^{-\beta}$, one can follow essentially the same steps we outlined in the discussion of the Ising model. Namely, the application of recursive counting using helical lattices and Chinese arithmetic comes through with no change at all. The differences are of a technical nature only, the conceptual ones.

Working with $h$ spins on a helix, the maximum number of configurations of the top layer is $q^h$. Since a single bit is no longer sufficient to keep the state of the individual spin, it would be more complicated to code the state of the top layer in a single word. Instead, we use several words to represent each top layer configuration. For example, for the $q = 3$ calculations we used two words per configuration while for $q = 8$ three words were required. It is also clear that now the analogue of Eq. (4) has $q$ terms, corresponding to the $q$ different possible values of the added spin.

We have computed the low temperature expansions for the energy, magnetization and susceptibility for the $q = 3$ model in $d = 2$ and $d = 3$ and the $q = 8$ model in $d = 2$. The
resulting series have been extensively discussed and analyzed in [7] and we do not repeat them here.

**Results and analysis**

Using these methods with the simple Ising model, we obtained the series for the average energy per bond given in Table (V). In Table (VI) we give the series through order 54 excited bonds for the magnetization and the magnetic susceptibility of the three dimensional model.

Table V. The low temperature expansion coefficients for the average energy per unit volume for the three, four, and five dimensional Ising model on a simple cubic lattice.

| $i$ | $e_i$ (3-d) | $e_i$ (4-d) | $e_i$ (5-d) |
|-----|-------------|-------------|-------------|
| 0   | 0           | 0           | 0           |
| 2   | 0           | 0           | 0           |
| 4   | 0           | 0           | 0           |
| 6   | 12          | 0           | 0           |
| 8   | 0           | 16          | 0           |
| 10  | 60          | 0           | 20          |
| 12  | -84         | 0           | 0           |
| 14  | 420         | 112         | 0           |
| 16  | -1,056      | -144        | 0           |
| 18  | 3,756       | 0           | 180         |
| 20  | -11,220     | 1,120       | -220        |
| 22  | 37,356      | -2,816      | 0           |
| 24  | -118,164    | 2,032       | 0           |
| 26  | 389,220     | 11,856      | 2,340       |
| 28  | -1,261,932  | -46,704     | -5,600      |
| 30  | 4,163,592   | 66,960      | 3,320       |
| 32  | -13,680,288 | 94,576      | 640         |
| 34  | 45,339,000  | -707,472    | 32,980      |
| 36  | -150,244,860| 1,545,120   | -122,220    |
| 38  | 500,333,916 | -148,656    | 145,540     |
| 40  | -1,668,189,060| -9,522,864 | -31,420     |
| 42  | 5,579,763,432| 30,130,576  | 454,860     |
| 44  | -18,692,075,820| -30,299,808| -2,483,360 |
| 46  | 62,762,602,860| -104,198,096| 4,560,440   |
| 48  | -211,062,133,044| 520,429,776 | -2,922,240 |
| 50  | 711,052,107,060| -918,744,400| 6,717,220  |
| 52  | -2,398,859,016,684|        |             |
| 54  | 8,104,930,537,260|        |             |
Table VI. The low temperature expansion coefficients for the average magnetization and magnetic susceptibility for the three dimensional Ising model on a simple cubic lattice.

| $i$ | $M_i$ | $\chi_i$ |
|-----|-------|----------|
| 0   | 1     | 0        |
| 2   | 0     | 0        |
| 4   | 0     | 0        |
| 6   | -2    | 1        |
| 8   | 0     | 0        |
| 10  | -12   | 12       |
| 12  | 14    | -14      |
| 14  | -90   | 135      |
| 16  | 192   | -276     |
| 18  | -792  | 1,520    |
| 20  | 2,148 | -4,056   |
| 22  | -7,716| 17,778   |
| 24  | 23,262| -54,392  |
| 26  | -79,512| 213,522 |
| 28  | 252,054| -700,362|
| 30  | -846,628| 2,601,674|
| 32  | 2,753,520| -8,836,812|
| 34  | -9,205,800| 31,925,046|
| 36  | 30,371,124| -110,323,056|
| 38  | -101,585,544| 393,008,712|
| 40  | 338,095,596| -1,369,533,048|
| 42  | -1,133,491,188| 4,844,047,090|
| 44  | 3,794,908,752| -16,947,396,000|
| 46  | -12,758,932,158| 59,723,296,431|
| 48  | 42,903,505,030| -209,328,634,116|
| 50  | -144,655,483,440| 736,260,986,208|
| 52  | 488,092,130,664| -2,582,605,180,212|
| 54  | -1,650,000,819,068| 9,074,182,912,884|

We will now give a brief analysis of our series to get results on the critical temperature and exponents. In the usual Dlog Pade (DlP) analysis [10], given a series expansion for $F(u)$ to $N$-th order, $F_N(u) = 1 + \sum_{i=1}^{N} f_i u^i$, (we will use the simplification that one can always normalize the series so that the constant term is unity), one computes coefficients for polynomials $Q_L(u) = \sum_{i=0}^{L} q_i u^i$ and $R_M(u) = 1 + \sum_{i=1}^{M} r_i u^i$, which satisfy,

$$Q_L(u)/R_M(u) = F'_N(u)/F_N(u)\quad (30)$$

to $O(u^N)$ with $L + M = N - 1$. 

---

20
The position $u_c$ of a singularity of $F$ of the form $F \sim A/|u-u_c|^{\zeta}$ will be approximated by the zeros of $R_M$. The exponent $\zeta$ is estimated by $\zeta = -Q_L(u_c)/R_M'(u_c)$.

In addition to DlP, we will also use the method of inhomogeneous differential approximants (IDA) introduced by Fisher and Au-Yang [11] (see also [12]). These are useful in handling singularities of the form,

$$F(u) = \frac{A(u)}{|u-u_c|^{\zeta}} + B(u)$$

where $A$ and $B$ are analytic in $u$. In this method, one computes coefficients for polynomials $Q_L(u)$, $R_M(u)$ and $S_J(u)$ which satisfy,

$$F_NQ_L + S_J = F_NR_M$$

(32)

to order $N$, with $L + M + J = N - 2$. Here the subscripts represent the highest order present in the given polynomials.

Note that for $S_J = 0$ one gets the usual Dlog Pade ratio from $Q_L/R_M$. It is easy to see that potential critical points $u_c$ are the zeros of $R_M$ and for each of these, the exponent $\zeta$ is again estimated as $\zeta = -Q_L(u_c)/R_M'(u_c)$.

In Fig. 2 we show the critical point $u_c$ and the exponent $\beta$ obtained from the magnetization series in Table (VI) using DlP and IDA analysis. The different points represent different values for the orders of the various polynomials used in the analysis. The critical value $u_c$ is most accurately known from Monte Carlo calculations and is shown as a vertical line. The thickness of this line represents the accuracy with which this number is known. As is clear, the DIP gives a $u_c$ quite far from the Monte Carlo value and the IDA results tend to scatter around it. If however, we take $u_c$ as given, we can calculate $\beta$ quite accurately from our results by interpolating the IDA results to the known $u_c$. Fitting a straight line to the points near $u_c$ in Fig. (2) gives $\beta = 0.289(1)$ where the errors are only the errors on the fit and ignore possible systematic effects from the unknown higher order terms in the series.

Similarly, the susceptibility series gives the results in Fig. 3. Now the results for the DIP and the IDA are mixed in together, in contrast to the magnetization series results (see above). Once again, the critical point is more accurately obtained from Monte Carlo
data, and, assuming that value, we find the exponent $\gamma = 1.281(1)$ from straight line fits to the data in the critical region.

Finally, we turn to the heat capacity, $C_v$, series. The results are shown in Fig. (4). The DilP line deceptively on a straight line which, if extrapolated to the Monte Carlo value for $u_c$ gives the wrong answer near $\alpha = 0.2$ as was already noticed in our earlier paper [13]. The IDA results on the other hand, are steeply varying in the region of $u_c$. If we take the three points from the $J = 0$ IDA data and fit them to a line, we get $\alpha = 0.128(1)$.

**Concluding remarks**

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 specific model. It is straightforward to introduce additional couplings, although this will increase memory needs. Some interesting possibilities for further exploration are gauge and coupled gauge-spin models in various dimensions. Changing boundary conditions should enable the study of interface properties. In Ref. [14] 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. Some work along these lines for gauge theories appears in Ref. [15]

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**Figure captions**

Fig. 1. Visualizing the helical lattice. All lattice points lying in the plane orthogonal to the vector $h$ are to be identified.

Fig. 2. The critical coupling and exponent $\beta$ obtained from the magnetization series for the three dimensional Ising model.

Fig. 3. The critical coupling and exponent $\gamma$ obtained from the magnetic susceptibility series for the three dimensional Ising model.

Fig. 4. The critical coupling and exponent $\alpha$ obtained from the energy series for the three dimensional Ising model.
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