Series expansions without diagrams

Gyan Bhanot,[1,2] Michael Creutz,[3] Ivan Horvath,[3,4] Jan Lacki,[2] and John Weckel[5]
[1]*Thinking Machines Corporation, 245 First Street, Cambridge, Massachusetts 02142*
[2]*Institute for Advanced Study, Princeton, New Jersey 08540*
[3]*Brookhaven National Laboratory, Upton, New York 11973*
[4]*Physics Department, University of Rochester, Rochester, New York 14627*
[5]*Physics Department, Princeton University, Princeton, New Jersey 08544*
(Received 5 March 1993)

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 diagrammatic approaches and is easily generalizable. We illustrate the approach using Ising and Potts models. We present low-temperature series results in up to five dimensions and high-temperature series in three dimensions. The method is general and can be applied to any discrete model.

PACS number(s): 02.30.Mv, 05.50.+q, 75.10.Hk, 02.70.−c

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. Reference [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. In this paper we extend these results to order 54. Reference [7] applied these methods to Potts models in two and three dimensions.

Being based on a transfer matrix, one might expect that the method only works well in low dimensions. We show, however, that this is partially compensated by several tricks which become more powerful in higher dimensions. Indeed, we present results for the Ising model in up to five dimensions.

This paper is primarily intended to explain these methods in more detail and explore extensions. In a recent paper Vohwinkel [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 σ_i taking the values ± 1. The energy of the system is

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

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

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

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

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

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

sider, 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

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

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,

$$P(E)=\sum_{I} p(E,I) \ . \tag{5}$$

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,

$$\langle E\rangle=\frac{\sum_E EP(E)}{Z}=2\left[u\frac{\partial}{\partial u}\right]\ln(Z) \ . \tag{6}$$

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

$$\langle E/N\rangle=\sum_j e_j u^j \ . \tag{7}$$

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 six excited bonds, and thus e_6 represents the first nontrivial term in our expansion. In our units, each excited bond has energy 2 and there are six 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. Reference [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

$$h_x<h_y<h_z \ . \tag{8}$$

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

$$n_x h_x + n_y h_y + n_z h_z = 0 \,. \tag{9}$$

Here n_i represents the number of steps in the ith direction. The length n of such a loop is

$$n = |n_x| + |n_y| + |n_z| \,. \tag{10}$$

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 10×10 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. Figure 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.

CANCELING 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. [2,3].

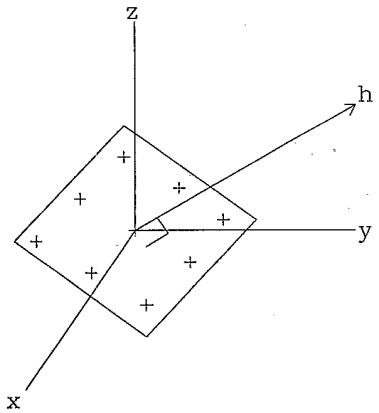

FIG. 1. Visualizing the helical lattice. All lattice points lying in the plane orthogonal to the vector **h** are to be identified.

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 $\mathbf{n}=(3,2,-4)$, 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 gives the series to the same order as a lattice with the smallest loops 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

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 **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)

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 canceling 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 such 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 canceled at the same time as the simple loops.) Denote the minimum distances between these three images as $d1$, $d2$, and $d3$. In most cases, the minimal way of flipping a set of spins to wrap around these three loops produces an energy of $(d-1)(d1+d2+d3-2)-2$, 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 $\mathbf{h}=(11,15,18)$ lattice, the fundamental loops have $\mathbf{n}=(0,6,-5)$, $(3,-1,-1)$ 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 $\mathbf{n}=(h_y,-h_y+1)$ 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 canceled.

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)
−4	(11,20,25,26)
−6	(15,18,25,26)
−16	(15,21,23,26)
−16	(7,20,24,25)
28	(14,15,23,25)
−21	(17,18,22,25)

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 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 [9].

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 $\mathbf{h}=(17,23,24)$ 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 three 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 lattice.

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

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

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

$$Z=\sum_{\{\sigma\}}\exp\left[-\beta E-H\sum_i\sigma_i\right]\ . \tag{12}$$

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

$$M=\langle\sigma_i\rangle=-\frac{1}{N}\frac{\partial}{\partial H}\ln Z \tag{13}$$

and the magnetic susceptibility

$$\chi=\frac{\partial}{\partial H}M\ . \tag{14}$$

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

$$P_k(E)=\sum_S S^k P(E,S)\ . \tag{15}$$

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

$$M=1-2\frac{\sum_E P_1(E)e^{-\beta E}}{NZ} . \quad (16)$$

Finally, from P_2 we can obtain the magnetic susceptibility

$$\chi=4\left[\frac{\sum_E [P_2(E)-P_1(E)^2]e^{-\beta E}}{NZ}\right] . \quad (17)$$

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

$$p'(E,S,I)=\sum_{I'} p(E-\Delta(I,I'),S-\Delta_s(I'),I') . \quad (18)$$

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,

$$p_k(E,I)=\sum_S S^k p(E,S,I) . \quad (19)$$

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

$$p_0'(E,I)=\sum_{I'} p_0(E-\Delta,I') , \quad (20)$$

$$p_1'(E,I)=\sum_{I'} p_1(E-\Delta,I')+\Delta_s(I)p_0(E-\Delta,I') , \quad (21)$$

$$p_2'(E,I)=\sum_{I'} p_2(E-\Delta,I')+2\Delta_s(I)p_1(E-\Delta,I') +\Delta_s^2(I)p_0(E-\Delta,I') . \quad (22)$$

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 the 2-point susceptibility $\mu_2=\langle x^2\sigma_x\sigma_0\rangle$. In the 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 ± 1. The partition function of Eq. (2) can be trivially rewritten

$$Z=\left[\frac{1+e^{-2\beta}}{2}\right]^{N_l}\sum_\sigma\prod_{\{i,j\}}[1+\sigma_i\sigma_j\tanh(\beta)] , \quad (23)$$

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 β 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 2. Thus we conclude

$$Z=2^N\left[\frac{1+e^{-2\beta}}{2}\right]^{N_l}\sum_k N(k)[\tanh(\beta)]^k . \quad (24)$$

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 as having "loose ends" or "dangling bonds." On adding a new site, we have the basic recursion relation

$$N'(k,I)=\sum_{I'} N(k-\Delta(I,I'),I') , \quad (25)$$

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 2 for whether the new x bond is selected times a factor of 2 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 is selected.

An immediate factor of 2 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 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 eight 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 22 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

$$F=\frac{\ln(Z)}{N_S}=\ln 2+\frac{N_L}{N_S}\ln\left[\frac{1+e^{-2\beta}}{2}\right]+\sum_k f_k[\tanh(\beta)]^k\,, \tag{26}$$

where N_Z and N_L denote the number of sites and links, respectively. To extract the coefficients f_k, it is somewhat easier to work with the analog of an expectation,

$$\langle k\rangle=\frac{\sum_k kN(k)}{\sum_k N(k)}\to N\sum_k kf_k\,. \tag{27}$$

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 kf_k themselves are always integers, while the f_k are not in general. We tabulated these numbers through order 22 in Table IV. These numbers are not new; for example they represent the same order as obtained in Ref. [3].

TABLE III. A combination of 16 lattices which gives the three-dimensional strong-coupling series through order 22. The first column represents the coefficient with which the lattice is to be weighted and the second gives the vector **h** which defines the lattices.

Coefficient	(h_x,h_y,h_z)
1	(12,17,20)
−1	(12,13,20)
2	(9,17,19)
−1	(15,16,19)
−1	(13,14,19)
2	(13,17,18)
1	(13,16,17)
−2	(8,15,17)
4	(5,15,16)
−4	(5,13,15)
−1	(10,11,12)
4	(5,10,12)
3	(5,7,12)
1	(9,10,11)
−4	(5,10,11)
−3	(5,6,11)

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

$$E=\sum_{\langle i,j\rangle}(1-\delta_{\sigma_i,\sigma_i})\,, \tag{28}$$

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

Writing the partition function in the form

$$Z=\sum_{E=0}^{dN}P(E)u^E\,, \tag{29}$$

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

TABLE IV. The coefficients for the strong-coupling series for the three-dimensional Ising model through order 22. The f_k are defined in the text.

k	kf_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
22	360 734 896 500

recursive counting using helical lattices and modular arithmetic comes through with no change at all. The differences are of a technical nature only, not conceptual.

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 analog 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 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.

CONCLUDING REMARKS

Using these methods with the simple Ising model, we obtained the series shown in Table V for the average energy per bond in three through five dimensions. The four-dimensional series are several terms shorter than have been presented in [10], but we include them to emphasize that our methods continue to work reasonably well in higher dimensions. As mentioned earlier, Ref. [8] has recently obtained several more terms for the three-dimensional model. In Table VI we give the series through order 54 excited bonds for the magnetization and the magnetic susceptibility of the three-dimensional model. These were obtained, as discussed above, from the moments of the state counts.

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. [11] 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. [12].

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 (3D)	e_i (4D)	e_i (5D)
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	χ_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	42 903 505 303	−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

ACKNOWLEDGMENTS

We thank Joseph Straley for discussions on turning finite-lattice partition functions into low-temperature series. We also thank David Atwood for discussions on the Chinese remainder theorem as a memory-saving trick. We thank T. Guttmann for a preliminary copy of Ref. [3]. We thank Professor M. E. Fisher for many useful comments. Some of the computations were done on the Cray-YMP at the Supercomputing Computations Research Institute at Florida State University, and some were done on the Cray computers at the National Energy Research Supercomputer Center, Livermore, CA. The order 54 three-dimensional Ising calculations were completed on Connection Machines at Thinking Machines Corporation. This work has been authored under Contracts No. DE-AC02-76CH00016 and DE-FG02-90ER-40542 of the U.S. Department of Energy. The work of G.B. was also partly supported by a grant from the Ambrose Monell Foundation. The research of J.L. was supported by the Swiss National Scientific Fund.

[1] K. Binder, Physica (The Hague) **62**, 508 (1972).
[2] I. G. Enting, Aust. J. Phys. **31**, 515 (1978).
[3] A. J. Guttmann and I. G. Enting, J. Phys. A **26**, 807 (1993).
[4] G. Bhanot, J. Stat. Phys. **60**, 55 (1990); G. Bhanot and S. Sastry, *ibid.* **60**, 333 (1990).
[5] M. Creutz, Phys. Rev. B **43**, 10 659 (1991).
[6] G. Bhanot, M. Creutz, and J. Lacki, Phys. Rev. Lett. **69**, 1841 (1992).
[7] G. Bhanot, M. Creutz, U. Glässner, I. Horvath, J. Lacki, K. Schilling, and J. Weckel, Phys. Rev. B **48**, 6183 (1993).
[8] C. Vohwinkel, Phys. Lett. B **301**, 208 (1993).
[9] M. Litzkow, M. Livny, and M. Mutka (unpublished).
[10] M. F. Sykes, J. Phys. A **12**, 879 (1979).
[11] M. Creutz, Phys. Rev. B **45**, 4650 (1992).
[12] R. Narayanan and P. Vranas, Nucl. Phys. **B330**, 608 (1990).