State counting and low-temperature series

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I present a simple numerical technique for evaluating the low-temperature expansion for discrete statistical systems. I begin with a recursive procedure on finite lattices to count the states of a given energy. Comparing these numbers on different lattice sizes, I extract coefficients for the infinite-volume series. I test the method with the three-dimensional Ising model, obtaining the expansion of the average energy through terms involving 34 excited bonds.

Some time ago Binder[1] presented a recursive procedure for finding exact solutions to the three-dimensional Ising model on a finite lattice. Recently Bhanot[2] and Bhanot and Sastry[3] have further investigated these methods and studied the analytic structure of the partition function in the context of finite-size scaling.

In this paper, I will adapt these recursive methods to extract the initial terms in the infinite-volume low-temperature expansion for the model. Here I obtain all terms involving 34 or less excited bonds. This series is slightly longer than previously presented,[4] but remains somewhat shorter than the more usual high-temperature expansions.[5] Nevertheless, the method pursued here is somewhat different and perhaps interesting in its own right.

The amount of work to evaluate either high- or low-temperature series grows exponentially with the order. For this reason, it is useful to mechanize as much of the calculation as possible. With the method presented here, no explicit reference to diagrams is needed, and the computer directly gives the desired coefficients. As with other methods, however, the work still grows rapidly with order, and it appears to require an unreasonable amount of computer time to extend the expansion beyond the orders presented here.

I will center my discussion on the three-dimensional Ising model, although the technique is also directly applicable to low-temperature expansions for any discrete statistical model. While I discuss the procedure in terms of a low-temperature series, one could, in principle, find the high-temperature expansion by working on the dual model. In particular, the low-temperature expansion for the three-dimensional Ising model is equivalent to the high-temperature series for the three-dimensional Z_2 lattice gauge theory. Unfortunately, I do not know how to generalize these ideas to models with continuous variables.

In Refs. 1 and 2 and below, exact values for the density of states are found for reasonably large lattices. For example, the largest system considered here has 162 spins. This system has $2^{162}=5.8\times10^{48}$ states. To enumerate them all would take astronomical time. The recursive method adapted from Ref. 1 allows one to find the exact number of states of any given energy. The 4^3 Ising model was solved exactly a few years ago by Pearson,[6] who made extensive use of symmetries to reduce the counting of the 2^{64} states to a feasible calculation. The methods presented here are not directly applicable to the calculation of Pearson because he used periodic-boundary conditions, which do not meld well with the recursive procedure.

For discussion I consider the Ising model on a finite three-dimensional simple cubic lattice. On each site i is a spin $s_i\in\{\pm1\}$. The energy of this system is

$$H=\sum_{i,j}(1-s_is_j)\ , \tag{1}$$

where the sum is over all nearest-neighbor pairs of spins. The partition function is

$$Z=\sum_{s_i=\pm1}e^{-\beta H}\ . \tag{2}$$

Here β represents the inverse temperature. I have normalized things so that two adjacent parallel spins contribute 0 to the energy, and two antiparallel neighbors contribute 2. I refer to those bonds connecting antiparallel neighbors as excited. While this model has not been solved analytically, it is generally accepted that there is a second-order phase transition at $\beta\sim0.2217$ separating a disordered phase from a magnetically ordered low-temperature phase.

Let $N(k)$ denote the total number of distinct states of our system which have k excited bonds. The partition function can then be rewritten

$$Z=\sum_k N(k)e^{-2\beta k}=\sum_k N(k)\mu^k\ , \tag{3}$$

where I have defined

$$\mu=e^{-2\beta}\ . \tag{4}$$

As the temperature decreases, β becomes large and μ becomes small. Thus at low enough temperature the first few terms in the expansion in Eq. (3) will be the largest. The numbers $N(k)$, then, are the coefficients in the low-temperature expansion for the partition function. On a finite system this expansion terminates at the order which equals the total number of bonds. On my 162-site model (to be specified later), the total number of bonds is 504, and thus no more than 504 integers are required to speci-

fy the solution.

Actually, rather than the partition function itself, we are more interested in the expansions for quantities such as the average energy per site. Thus I define

$$E=\frac{1}{VZ}\sum_{s_i=\pm 1} He^{-\beta H}=\frac{2}{V}\mu\frac{\partial}{\partial\mu}\ln(Z)\ . \tag{5}$$

Here V denotes the number of sites in our system; I divide this out so that E will have a finite infinite-volume limit. Given the coefficients $N(k)$, it is straightforward to rearrange the series to give an expansion for the energy itself

$$E=\sum_k E_k\mu^k\ . \tag{6}$$

The coefficients E_k should have a finite limit as the system volume goes to infinity. It is these numbers that I pursue in the following. I note in passing that it is not difficult to show that these infinite volume coefficients are all integers.

I begin by reviewing the recursive procedure for determining the numbers $N(k)$. Starting with a small lattice, I add additional spins to form a larger lattice. I build my lattice up starting from a single layer in the first two dimensions, and add spins to build up successive layers on top. In this process, I need to know the number of states of a given energy and with given spins on the top layer, to which I attach the additional ones. I define a counting index $M(k,S)$ which denotes the number of states with k excited bonds and with a specified set S of exposed spins on the top. For a partially filled layer at height z, the spins in S consist of the additional spins on this layer and the still uncovered spins of the previous layer. For our hypercubic lattice the number of spins in the set S is the number of spins in one transverse plane of the system and is constant throughout the construction.

Now consider adding one additional spin to the lattice. Denote the counting index as M'. The added spin covers one of the old ones, which can be either parallel or antiparallel to the added one. The recursion relation giving the count is

$$M'(k,S)=M(k-\Delta,S)+M(k-\Delta',S')\ . \tag{7}$$

Here the first term represents the case when the covered spin has the same value as the additional one, and thus the top spins are the same. The second term comes from when the covered spin is antiparallel to the additional one, and thus the covered spins S' differ from S only in having the spin at the location of the additional one flipped. The numbers Δ and Δ' denote the number of excited bonds appearing in the addition of the spin. These shifts are easily calculated, although the details of their values depend on which spin is being added and the desired boundary conditions of the system. To initiate the procedure, enumerate explicitly the states for a single layer of the system. In this case all the values in the array M are 0 unless the number of excited bonds in the set S itself is exactly k, in which case $M(k,S)=1$. The overall scheme reduces the enumeration of the 2^V states of the system to a loop of length $V\times 2^{V_T}$, where V_T denotes the number of spins on a transverse slice of our lattice.

For large systems, the counts become quite large integers, and for an exact evaluation one may need to use high-precision integer arithmetic. For the results presented here, however, I consider systems small enough that double precision floating point numbers contain all needed counts without any roundoff error. Nevertheless, the recursion always adds positive numbers; thus, if one only needs approximate results, floating point calculations will not accumulate excessive roundoff errors.

Note that with this method, the boundary conditions in the transverse direction are quite arbitrary. It is, however, quite awkward to obtain periodic boundaries in the third coordinate. To build up a periodic lattice, one would need to keep the counts for all possible values of the bottom plane as well as the top. Then the final lattice can be closed up with periodic boundaries. However, this requires substantially greater storage and computer time.

To extract the infinite-volume low-temperature series from these counts, I compare two different lattice volumes. Taking the expansions for the total energy on each of these lattices, I take the difference of these series and divide by the change in the volume. This will give the correct series up to an order where finite-volume effects set in. These can come from several sources.

First, if the surface of the lattice changes between the two systems, then I could have surface effects. To avoid this I take cyclically periodic boundaries in the transverse direction. Thus all surfaces are at the longitudinal ends of the lattice and are invariant as I lengthen the lattice in that direction. To make the longitudinal ends appear just as a cold continuation of the lattice, I place layers of spin-up spins above and below the system.

Second, if I consider exciting an ordered lattice, some excitations will involve groups of spins which can tell that the lattice is indeed finite. Since the algorithm easily allows us to make the longitudinal direction as long as needed, these problems are serious only for excitations sensitive to the finite transverse size. If our transverse system has each site at least n steps away from its periodic image, any such excitation will involve at least $2n$ excited longitudinal bonds. Here a simple trick using the symmetry of an infinite lattice under permutation of the axes greatly extends the order to which we can push the series. Introducing separate couplings for the x, y, and z directions, we consider expanding the energy simultaneously in the three couplings. In the infinite-volume limit, the coefficients in this series will be invariant under permutation of these directions. Thus we can calculate the energy series on a finite lattice, and for a particular term, replace it with one corresponding to the smallest number of excited longitudinal bonds. This will make the series correct as long as some direction involves less than $2n$ excited bonds. In this way we obtain the final series for the symmetric lattice up to order $6n$.

Clearly it is desirable to have each spin as far as possible from its image. With a simple periodic n by n lattice, we have $V_T=n^2$ and can obtain the series up to order $6n$. I now introduce a variation on helical boundary conditions wherein a site is separated from its image by at least

n spins in all directions, but the total number of spins is considerably less than n^2.

A two-dimensional lattice with helical boundary conditions can be thought of as a ring of V_T spins where the neighbors of each spin are the two adjacent spins and two more spins x steps up and down the chain. One turn of the helix has length x, and the helix starts repeating after V_T spins. Conventionally such boundary conditions are quite convenient for vectorization, as neighbors are always a fixed distance away in computer memory. Usually V_T is taken to be a multiple y of x, so we can loosely speak of an x by y lattice. Here, however, it turns out to be convenient to have a fractional number of helical turns in one period of the entire lattice. Indeed, I will take $y=V_T/x$ to be near a half integer.

On such a lattice, finite-size effects are related to closed paths which wrap in some way around the helix. For example, one such path is to jump to the next turn in the helix, and then return to the starting point in x single steps along the helix. This will involve $x+1$ bonds. Another closed path is to keep jumping forward the integer part of y turns of the helix, and then do a few additional single steps to return home. This requires $[y]+(V_T-[y]x)$ steps. Here the square brackets mean the greatest integer less than or equal to y. A similar path does one more jump along the helix spins before returning in single steps, and has $[y+1]+([y+1]x-V_T)$ steps. If I wish to obtain results to comparable order to those from an n by n periodic lattice, I must have all these possible paths with length greater or equal to n. The minimal solution to these constraints is not unique, but a simple choice is $V_T=[(n^2+1)/2]$ and $x=2[(n+1)/2]-1$. For some explicit examples, a helix of five spins with three spins per turn mimics a 3 by 3 periodic lattice, eight spins with three per turn mimics a 4 by 4 lattice. For short, I will denote these as 3 by $\frac{5}{3}$ and 3 by $\frac{8}{3}$ lattices. Finally, 5 by $\frac{13}{5}$, and 5 by $\frac{18}{5}$ lattices give results to the same order as 5 by 5 and 6 by 6 periodic lattices, respectively. The latter 18-site lattice is used for the results presented below, and gives the infinite-volume low-temperature series through 34th order.

As computer time and storage requirements grow exponentially with the transverse volume, this use of peculiar boundaries gives a substantial saving. For example, consider the 18-site lattice arranged helically with a period of 5. This gives the series correct through 34th order in μ. A simple periodic lattice would require 6×6 sites for the same order; the elimination of 18 spins saves a factor $2^{16}=65\,536$ in memory. This order would have been impossible without this trick. On the other hand, the next size lattice, which gives the same results as a 7 by 7 periodic system, has 25 sites, and is probably impractical to work with.

The above method works quite well for smaller lattices, but as the size increases it requires rather large amounts of memory. If a transverse slice has V_T spins and we are interested in keeping track of all lattices containing up to k excited bonds, then we need to store $2^{V_T+1}k$ variables, where the extra factor of 2 is because we need both the old and new counts for the recursion.

With periodic transverse boundaries, a small change in the procedure substantially reduces the memory requirements but at a fairly large penalty in computer time. Instead of adding a single spin at a time, consider adding a whole layer. Then the inner loops become much longer, being over both all values of the layer and all values of the covered one. Nevertheless, by adding the whole layer at once, I can make extensive use of symmetries in this layer. In particular, with my transverse helical periodic boundaries, the counts for some given set of top-layer spins will be the same for any cyclic permutation of this layer. It is also the same for the bits of the top layer taken in reverse order. Thus we only need to store the count for a standard form for each set of possible layers related by one of these symmetry operations. This saves a factor of somewhat less than $2V_T$ in memory. (The saving is somewhat less because some configurations of the top layer are invariant under certain symmetries.) For example, with the 18-site transverse lattice discussed below, instead of having to keep counts for $2^{18}=262\,144$ top layers, I only need keep track of 7685 standard forms.

One final trick saves an additional factor of nearly 2 in computer time. Consider a given longitudinal size z and suppose I have obtained the number of states for any given energy and all possible top layers for the lattice. I can turn this lattice upside down on top of itself and then loop over the top plane, which is now in the middle of a sandwich. In this way I find the number of states on a lattice of longitudinal size $2z-1$. Using the counts from the previous layer for the top of the sandwich, I obtain the final counts for a lattice of size $2z-2$.

I have tested these methods on the simple three-dimensional Ising model. Working on an 18-site helical lattice with period 5, I built up on a cold boundary five layers in the longitudinal direction. Using the above tricks, I obtained the state counts for longitudinal sizes up to 9 and including up to 34 excited bonds. Programmed in *C*, this calculation required approximately a day on a Sun Microsystems SPARC station SLC. The time required grows rapidly with system size; to obtain the series through 28 excited bonds on a 5 by $\frac{13}{5}$ by a 7-site system only requires about two minutes.

With the boundary conditions chosen, only states with an even number of excited bonds appear in the final count. At intermediate stages in the calculation, there are configurations with odd numbers of longitudinal excitations. The single zero-energy state is simply the state with all spins up. This state is nondegenerate because of the cold walls. The next states have six excited bonds and correspond to a single spin down in a sea of up spins. The number of such states is just the number of sites on the lattice.

I then manipulated these counts to obtain the series for the average energy. Taking the difference of these expansions for two longitudinal volumes, and then dividing by the change in transverse volume gave the low-temperature series for the average energy per spin. To take advantage of the above-mentioned symmetry under permutation of directions, I evaluated this series while keeping separate track of excited bonds in the three

different directions, and restricted the counts to consider only up to ten excited longitudinal bonds. Combining these counts gave the final series coefficients in Table I. One simple consistency check on these numbers was to repeat the calculation comparing longitudinal size $z=9$ with 8, and $z=8$ with 7. Comparing $z=7$ with $z=6$ gave finite-size corrections at 34th order, as expected.

Note that the series starts out alternating in sign. The sign of the 12th order term can be understood because there are no connected clusters of flipped spins with energy 12; so, this coefficient is entirely due to the excluded volume available to two isolated flipped spins of energy 6 each. As expected, all the coefficients are integers.

In Ref. 4 all excitations of up to 11 flipped spins were studied. Their analysis agrees with the numbers in this table, and by adding to their treatment the rather simple enumeration of the 12-spin diagram with 32 excited bonds, all numbers in Table I are verified.

To summarize, I have presented a simple mechanical technique for evaluating the coefficients for low-temperature expansions in discrete statistical models. The method requires no explicit diagrammatic analysis. I illustrated the method on the series for the average energy per site of the three-dimensional Ising model. With a modest amount of computer time, I found this expansion to 34th order in $e^{-2\beta}$. This series could be manipulated in standard ways to find the specific heat or free energy, and summation methods could be used to determine properties of the critical point for the model. As the series is somewhat shorter than those available for the strong-coupling limit, this will presumably not add much to our knowledge of this transition. Nevertheless, the technique is simple to implement and applicable to many other models.

TABLE I. The coefficients of the low-temperature series for the average excitation energy per site for the three-dimensional Ising model on a simple cubic lattice.

order k	E_k
0	0
2	0
4	0
6	12
8	0
10	60
12	−84
14	420
16	−1056
18	3756
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

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