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Transfer matrix for the restricted canonical and microcanonical ensembles

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The numerical transfer matrix for the partition function of discrete lattice models is generalized to allow the calculation of the density of states $\Omega(E)$, and the restricted density of states $\Omega(E,M)$. Given $\Omega(E,M)$ the partition function is expressed as a polynomial in the variables $x=e^{\beta h}$ and $y=e^{-\beta}$. These algorithms are illustrated with calculations for the Ising model on finite square lattices. The zeros of the partition function are examined in both the complex x and y planes. Finite size scaling analysis of the zeros leads to very accurate estimates for the critical temperature and critical exponents.

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INTRODUCTION

In an important paper Binder [1] showed that the partition function for discrete lattice models, and in particular the Ising model, can be calculated exactly by the numerical transfer matrix. In a more recent paper, Bhanot [2] devised a method which uses the Binder algorithm to construct the exact density of states, $\Omega(E)$. This is done by evaluating the partition function for several rational values of the temperature parameter $y=e^{-\beta}$, and then solving a set of coupled equations for $\Omega(E)$.

In this paper I present a method of determining the density of states directly by a transfer matrix. The method is then generalized to allow the calculation of the restricted density of states, which is simply the number of states with fixed energy and fixed order parameter (magnetization). Given the restricted density of states the free energy, internal energy, entropy, specific heat, magnetization, and susceptibility can be expressed as polynomials in x and y. Finally, a hybrid algorithm which requires much less computer memory is presented which gives the partition function at a given temperature for all values of the magnetization. The algorithms presented here can be applied to any lattice with equally spaced energy levels (e.g., the q-state Potts model); here the Ising model is used for illustrative purposes and because it requires the least computer resources.

The Hamiltonian for the Ising model with exchange constant $J=1$ is

$$H=\tfrac{1}{2}\sum_{\langle i,j\rangle}(1-S_iS_j), \tag{1}$$

where $S_i=\pm 1$ and $\langle ij\rangle$ label nearest neighbor sites on a two or three dimensional lattice. As defined in (1) the energy ranges from 0 to N_b in unit steps [3] where N_b is the number of bonds on the lattice.

The density of states is

$$\Omega(E)=\mathrm{Tr}\,\delta(E-H), \tag{2}$$

where $\delta(E-H)$ is the Kronecker delta and the trace is over all the states of the system. The density of states takes on only integer values, and given $\Omega(E)$ the partition function for inverse temperature β is a polynomial in $y=e^{-\beta}$,

$$Z(y)=\sum_{E=0}^{N_b}\Omega(E)y^E. \tag{3}$$

If one is interested in the magnetic properties of the model one can define the restricted density of states,

$$\Omega(E,M)=\mathrm{Tr}\left[\delta(E-H)\,\delta\left(M-\tfrac{1}{2}\sum_i(1-S_i)\right)\right]. \tag{4}$$

The magnetization M defined in (4) ranges from 0 for the ferromagnetic spin up state to N_s for the ferromagnetic spin down state in steps of two. N_s is the number of spins on the lattice. The partition function in a magnetic field, h, is then

$$Z(x,y)=\sum_{M=0}^{N_s}\sum_{E=0}^{N_b}\Omega(M,E)x^My^E, \tag{5}$$

where $x=e^{\beta h}$.

MICROCANONICAL TRANSFER MATRIX FOR THE DENSITY OF STATES

For simplicity consider the transfer matrix in two dimensions; the generalization to higher dimensions is straightforward. The spins are located at the sites of a square lattice of size $L\times N$ with periodic boundary conditions in the transverse direction (length L) and open boundaries in the longitudinal direction (length N). For the first row of L spins we define

$$\omega^{(1)}(E;S_1,\ldots,S_L)=\delta\left(E-\tfrac{1}{2}\sum_{i=1}^{L}(1-S_iS_{i+1})\right). \tag{6}$$

The first step in the transfer matrix is to introduce the interaction between a spin in the first row with the corresponding spin in the second row and then trace over the spin in the first row. For the first spin we have

$$\tilde{\omega}(E;S_1',S_2,\ldots,S_L)=\sum_{S_1=\pm 1}\omega^{(1)}(E-\tfrac{1}{2}(1-S_1'S_1);S_1,S_2,\ldots,S_L). \tag{7}$$

Note that the new function defined in (7) has exactly the same number of arguments as in (6); the amount of memory needed in each step of the calculation remains fixed.

This process is repeated for each of the spins in the first row in turn; once all the spins in the first row have been traced over we are left with a function only of the spins in the second row. At this point the interactions between spins in the second row are added to the energy giving

$$\omega^{(2)}(E;S_1',S_2',\ldots,S_L')=\tilde{\omega}\Big(E-\tfrac{1}{2}\sum_{i=1}^{L}(1-S_i'S_{i+1}');S_1',S_2',\ldots,S_L'\Big). \tag{8}$$

The entire process can now be repeated until finally we have a function of the spins in the last (Nth) row. The density of states is given by tracing over the spins in the Nth row,

$$\Omega(E)=\sum_{S_1=\pm1}\sum_{S_2=\pm1}\cdots\sum_{S_L=\pm1}\omega^{(N)}(E;S_1,S_2,\ldots,S_L). \tag{9}$$

RESTRICTED MICROCANONICAL TRANSFER MATRIX

The above procedure can be modified in a straightforward way to calculate the restricted density of states, (4). For the first row one has, instead of (6),

$$\omega^{(1)}(M,E;S_1,\ldots,S_L)=\delta\Big(M-\tfrac{1}{2}\sum_{i=1}^{L}(1-S_i)\Big)\,\delta\Big(E-\tfrac{1}{2}\sum_{i=1}^{L}(1-S_1S_{i+1})\Big). \tag{10}$$

The spins in the first row are traced over in sequence just as in (7) leading to a new function of the spins in the second row;

$$\tilde{\omega}(M,E;S_1',S_2,\ldots,S_L)=\sum_{S_1=\pm1}\omega^{(1)}(M-\tfrac{1}{2}(1-S_1'),E-\tfrac{1}{2}(1-S_1'S_1);S_1,S_2,\ldots,S_L). \tag{11}$$

Once all the spins in a row have been traced over, the function for the next row is completed as in (8)

$$\omega^{(2)}(M,E,S_1,\ldots,S_L)=\tilde{\omega}\Big(M,E-\tfrac{1}{2}\sum_{i=1}^{L}(1-S_iS_{i+1});S_1,\ldots,S_l\Big) \tag{12}$$

and the restricted density of states is given by

$$\Omega(M,E)=\sum_{S+1=\pm1}\cdots\sum_{S_L=\pm1}\omega^{(N)}(M,E,S_1,\ldots,S_L). \tag{13}$$

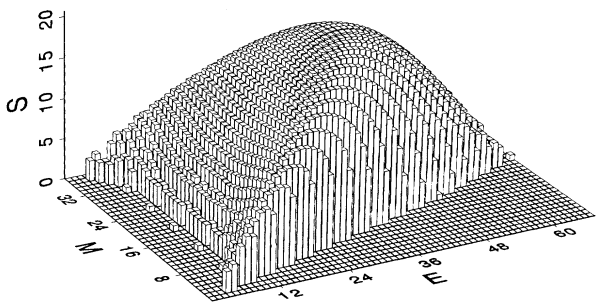

FIG. 1. the restricted entropy $S(M,E)=\ln\Omega(M,E)$ for a 6×6 Ising model with open boundary conditions.

Figure 1 shows the complete histogram for the entropy $S(M,E)$ for $L=6$. Note that at low energies the density of states exhibits a double maximum for magnetizations different from zero. This is reflected in the free energy, which exhibits a double minimum characteristic of the ordered phase.

The partition function of the Ising model as a function of both temperature and magnetic field can now be expressed as a polynomial in the variables x and y as in (5). However, if one is only interested in the critical behavior of the model as a function of the magnetic field, it is sufficient to examine the zeros of the partition function at the critical value for the temperature parameter, y_c, which can be determined in the usual way from the microcanonical transfer matrix.

RESTRICTED CANONICAL TRANSFER MATRIX

As a final variation [4] of the transfer matrix, the Binder algorithm can be modified to give the partition function at a fixed temperature for all values of the magnetization. For each state of the first row of spins we define

$$\omega^{(1)}(M,y;S_1,\ldots,S_L)=\delta\Big(M-\tfrac{1}{2}\sum_{i=1}^{L}(1-S_i)\Big)y^{E[\{S\}]}, \tag{14}$$

where $E[S]$ is the energy contributed by the bonds in the first row as in (6).

The spins in the first row are summed over as before according to the modified rule

$$\tilde{\omega}(M,y;S_1',S_2,\ldots,S_L)=\sum_{S_1+\pm1}\omega^{(1)}(M-\tfrac{1}{2}(1-S_1'),y;S_1,\ldots,S_l)y^{(1-S_1'S_1)/2}. \tag{15}$$

When all the spins in a row have been summed, the contribution to the restricted partition function from the bonds in the second row is taken into account exactly as in the Binder algorithm;

$$\omega^{(2)}(M,y;S_1',\ldots,S_L')=\bar{\omega}(M,y;S_1',\ldots,S_L')y^{E[\{S'\}]}. \tag{16}$$

Finally, when only the last row of spins remains, the restricted partition function is given by

$$\Omega(M,y)=\sum_{S_1=\pm 1}\cdots\sum_{S_L=\pm 1}\omega^{(N)}(M,y;S_1,\ldots S_L) \tag{17}$$

and the full partition function is now a polynomial in x,

$$Z(x,y)=\sum_{M=0}^{N_s}\Omega(M,y)x^M. \tag{18}$$

DISCUSSION

The scaling of the computational complexity of the various algorithms presented here can be compared with the Binder algorithm. For an n-component model in d dimensions the memory required by the Binder algorithm is proportional to $nn^{L^{(d-1)}}$ and the time required scales as $nN_sn^{L^{d-1}}$. For the three variations of the transfer matrix considered here both the time and memory increase by a factor of N_b for the microcanonical transfer matrix, by N_s for the restricted canonical transfer matrix, and by $N_s\times N_b$ for the restricted microcanonical transfer matrix. It is interesting to note that the computational complexity of Bhanot's algorithm and the microcanonical transfer matrix, both of which yield the density of states, scale in the same way with the size of the system. The restricted microcanonical transfer matrix requires the most computational resources, and this limits its application to relatively small lattices.

Using the microcanonical transfer matrix, the density of states for Ising models on $L\times L$ square lattices for $3\leq L\leq 13$ have been calculated. We know from the famous theory of Yang and Lee [5] that the critical behavior of the model arises in the limit $L\to\infty$ when the zeros of the partition function close in on the physical part of the real axis. The scaling of the dominant zero, y_0, follows from the finite size scaling form for the free energy;

$$\mathrm{Re}(y_0)=y_c+AL^{-1/\nu}(1+a_1L^{-\omega}+a_2L^{-2\omega}+\cdots) \tag{19}$$

and

$$\mathrm{Im}(y_0)=BL^{-1/\nu}(1+b_1L^{-\omega}+b_2L^{-2\omega}+\cdots). \tag{20}$$

In (19) and (20) ω is a correction-to-scaling exponent, A, B, $\{a_k\}$, and $\{b_k\}$ are constants, and ν is the correlation length exponent.

Following Bhanot, these data can be analyzed by the method of Bulirsh and Stoer [6,7] (BST). The BST estimate with $\omega=1.000$ for y_c is 0.414 213 583(6) which should be compared with the exact value $\sqrt{2}-1=0.414\,213\,562\ldots$. One can also define a sequence of estimates for the leading scaling exponent, ν,

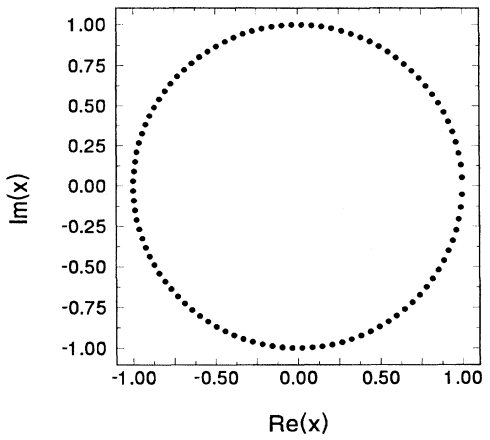

FIG. 2. Zeros of the partition function in the complex x plane for a 10×10 Ising model with open boundary conditions.

$$\nu(L)=\frac{\ln[(L+1)/L]}{\ln(\{\mathrm{Re}[y_0(L+1)]-y_c\}/\{\mathrm{Re}[y_0(L)]-y_c\})}. \tag{21}$$

Applying the BST procedure (again with $\omega=1$) to these data yields $\nu=1.000\,000\,7(5)$ which should be compared with the exact value $\nu=1$.

By a theorem of Yang and Lee [5] we know that the zeros of the partition function in the complex x plane lie on the unit circle. Figure 2 shows that zeros of the partition function for $y=y_c$ for $L=10$.

At the critical value $y=y_c$ the partition function for an infinite lattice is nonanalytic at $x=1$ ($h=0$). From the scaling form of the free energy the argument [8] of the dominant zero in the complex x plane approaches the real axis as

$$\theta(L)=CL^{-y_h}(1+C_1L^{-\omega}+C_2L^{-2\omega}+\cdots), \tag{22}$$

where for the Ising model in two dimensions $y_h=\frac{15}{8}$.

The restricted microcanonical transfer matrix was used to calculate $\Omega(M,E)$ for sizes $3\leq L\leq 10$. The zeros of the partition function in the complex x plane were then calculated for $y=y_c$. For lattices of sizes $11\leq L\leq 13$ the restricted ca-

TABLE I. Arguments of the dominant zero in the complex x plane for lattices of size $3\leq L\leq 13$ ($T=T_c$).

L	θ_0
3	0.471 998 042 060
4	0.287 611 162 550
5	0.188 399 320 772
6	0.135 505 282 011
7	0.102 460 660 627
8	0.080 370 500 991
9	0.064 840 294 164
10	0.053 487 453 592
11	0.044 925 672 320
12	0.038 302 191 885
13	0.033 068 293 166

nonical transfer matrix with $y=y_c$ was used to find $\Omega(x,y_c)$ and again the zeros were calculated. The arguments of the zero closest to the critical point for $3\leq L\leq 13$ are listed in Table I.

Estimates for the magnetic scaling exponent can be calculated as in (21) and the BST analysis with $\omega=1.000$ yields the estimate $y_h=1.876(2)$ which agrees very well with the exact result.

CONCLUSIONS

The Binder algorithm is easily generalized to allow the calculation of the density of states and the restricted density of states. Given $\Omega(M,E)$, the partition function at any temperature and in an arbitrary magnetic field can be evaluated, and it is possible to study the analytic properties of the partition function in both the complex y (temperature) and x (magnetic field) planes. In addition, the free energy, specific heat, order parameter, and susceptibility are also given for any temperature and magnetic field; the restricted density of states yields a complete thermodynamic description of the system.

ACKNOWLEDGMENTS

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[1] K. Binder, Physica **62**, 508 (1972).

[2] G. Bhanot, J. Stat. Phys. **60**, 55 (1990).

[3] The energy of the Ising model with periodic boundary conditions is quantized in units of $2J$. However, with open boundary conditions the spins at the edges of the lattice have only three neighbors leading to states with energies which are odd multiples of J.

[4] It is also possible to calculate the weighted density of states $\Omega(x,E)$ by transfer matrix. This variation seems to be of less utility than those presented here.

[5] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952); **87**, 410 (1952).

[6] R. Bulirsch and J. Stoer, Num. Math. **6**, 413 (1964).

[7] M. Henkel and G. Schutz, J. Phys. A **21**, 2617 (1988).

[8] The Yang-Lee theorem constrains the zeros to lie on the unit circle so that in the limit $L\rightarrow\infty$ $\theta_0(L)\simeq L^{-y_h}$. This is unlike the situation in the complex y plane, where the real and imaginary parts approach the critical point along a line with finite slope.