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Partition function of the Ising model on the periodic $4\times4\times4$ lattice

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The exact partition function of the Ising model on a periodic $4\times4\times4$ simple cubic lattice is presented. The methods used in deriving this quantity, based on low-temperature series, are discussed. The zero-field partition function is analyzed to locate its zeros in the complex plane, and these results are discussed.

I. INTRODUCTION

The Ising model, which has a long history of calculations of every imaginable sort,[1] is defined by the partition function

$$Z(\beta,h)=\sum_{(S_i)=\pm1}\exp\left[\beta\sum_{\mathrm{NN}}(S_iS_j-1)+\sum_i h_i(S_i-1)\right]. \quad (1.1)$$

For studying critical behavior, two very successful techniques are series expansions and the renormalization group. For gaining understanding of the analytic structure of the free energy considered as a function of β and h, these methods are not always very useful. The renormalization group describes the behavior in the scaling region of a critical point, while series tend to be dominated by nearby singularities. A more promising approach may be the study of the exact behavior of the free energy on finite lattices. Roughly, one may argue that except very near to a "critical point," the finite system behaves very much as the infinite system and that this behavior should extend to the complex plane.

For this reason it is interesting to study the behavior of finite Ising lattices. There already exist some results in two dimensions on square lattices[2] and in three dimensions on simple cubic lattices.[3] In the latter case, these extend up to $3\times3\times3$, and $3\times3\times n$ should be possible soon.[4] It is the purpose of this paper to present a calculation of the partition function of the $4\times4\times4$ periodic, simple cubic Ising lattice, and some preliminary results on its analytic structure. It is felt that these results, although limited in scope, merit presenting since they represent one of the largest three-dimensional systems for which exact results are known and may be of use to others.

In Sec. II the computational techniques that have been used are described. Since they are essentially an adaptation of the standard methods for generating low-temperature series,[5] not much detail is necessary. Then the main results of this paper will be given. The sheer volume of data generated precludes publishing all of it. Rather, the most useful results are presented, and the remainder will be made available upon request. What has been computed are all of the complete partial generating functions or "codes." From these have been derived the complete set of high-field polynomials and the zero-field partition function, which is a polynomial of 96th order in $u=e^{-4\beta}$. Here I will give only the zero-field partition function, and defer the high-field polynomials to another paper in which discussion of the field dependence of the zeros of the partition function is planned. Finally, I present an analysis of the zero-field partition function in the complex plane and compare this to the currently known structure for the infinite volume limit.

II. DERIVATION OF THE PARTITION FUNCTION

For the 4^3 Ising lattice there are 2^{64} or about 2×10^{19} distinct spin states. When translation invariance and cubic symmetry are taken into account, there still remain of the order of 10^{16} separate spin configurations to count. This would be impossible by direct enumeration. There is a method that has been exploited in deriving low-temperature series[5] which reduces the amount of labor dramatically. This is the code method or shadow-lattice method. Here, one separately sums over even- and odd-site spins. Since all odd-site spins couple only to even-site spins, for a given configuration of even-site spins the sum over each odd-site spin factorizes, and the resulting contribu-

tion to the partition function is a product of 32 binomial factors. The full expansion of these gives the 2^{64} states, but only 2^{32} (even) spin configurations need be enumerated. There is a simplification due to the fact that the odd-site spins are coupled to the sum of their six even-site neighbors. Thus there can only be seven distinct binomial factors, depending on whether the number of neighbors with the value -1, or flipped spins, is 0 through 6. The partition function is then expressed in terms of a sum of factorized polynomials of the form

$$b_0^{n_0} b_1^{n_1} b_2^{n_2} b_3^{n_3} b_4^{n_4} b_5^{n_5} b_6^{n_6} , \tag{2.1}$$

where n_i is the number of odd sites with i flipped even neighbors. Clearly we have

$$n_0+n_1+n_2+n_3+n_4+n_5+n_6=32 , \tag{2.2}$$

and

$$(n_1+2n_2+3n_3+4n_4+5n_5+6n_6)/6=n_e , \tag{2.3}$$

where n_e is the total number of flipped even spins in a given configuration. It is convenient to introduce the variables

$$y_\pm=\exp(-2h_\pm) , \tag{2.4}$$

and

$$u=\exp(-4\beta) , \tag{2.5}$$

where $h_\pm$ is a uniform field on the even or odd sites, respectively. The partition function (1.1) has been normalized so that when all of the spins have the value $+1$, one obtains 1. For each even- (odd-) site spin flipped to -1, one obtains a factor $y_{+(-)}$. For each pair of neighboring spins for which $S_iS_j=-1$, one obtains a factor $\sqrt{u}$; however, since flipping any spin changes an even number of pairs, Z depends only on u. It is convenient to associate to each even flipped spin a factor u^3. Then one obtains an expression for the partition function solely in terms of the n's:

$$Z=\sum_{(n_i)} C(n_0,n_1,\ldots,n_6)(u^3y_+)^{n_e} \sum_i ni=32 \times \prod_{i=0}^{6}(1+y_-u^{3-i})^{n_i} , \tag{2.6}$$

where the C's are non-negative integers. It is convenient to represent all of the algebraic factors in (2.6) by a special symbol or code from which the method derives its name. Then we may write compactly

$$Z=\sum_{(\vec{n})} C(\vec{n})[n_0,n_1,\ldots,n_6] . \tag{2.7}$$

Given the coefficients C, it is a straightforward matter to evaluate Z for given β,h_+,h_- or to extract high-field polynomials or the zero-field partition function itself. The procedure to determine the C's is to enumerate each even-site spin configuration and count for each odd site the number of flipped even neighbors. The number of odd sites of each type are the n_i. Finally, 1 is added to the appropriate count $C(n)$. A modest amount of work may be saved by exploiting various symmetries. The cubic symmetry (the order of the group is 48) is most important, saving an average factor of about 30 in the number of states to be enumerated. Translation invariance and Z_2 spin symmetry each save another factor of about 2. (Translation invariance saves less than one might think because it is difficult to generate only translationally inequivalent configurations and determine the symmetry factor for each.) The number of configurations that need to be enumerated is thus $\sim 2^{32}/120$, or about 30 million. The program running on a CDC 7600 required about 50 μsec to analyze each configuration for a total time of around 1500 sec. The enumerations were performed separately for each n_e. Owing to Z_2 spin symmetry, only $0\le n_e\le 16$ need be computed explicitly. The cases $17\le n_e\le 32$ can be obtained from the former by inverting the order of the n's. The number of distinct codes for

TABLE I. Number of distinct codes for n_e flipped even spins.

n_e	Number of codes
0	1
1	1
2	2
3	4
4	10
5	19
6	40
7	79
8	139
9	224
10	354
11	511
12	712
13	913
14	1076
15	1186
16	1240

TABLE II. Coefficients of the zero-field partition function in $u=e^{-4\beta}$.

n	Z_n	n	Z_n	n	Z_n
0,96	2	1,95	0	2,94	0
3,93	128	4,92	0	5,91	384
6,90	3 648	7,89	1 920	8,88	20 448
9,87	71 680	10,86	125 952	11,85	537 600
12,84	1 445 440	13,83	3 756 288	14,82	11 173 440
15,81	29 955 072	16,80	79 741 908	17,79	214 759 680
18,78	564 284 736	19,77	1 466 972 160	20,76	3 794 966 880
21,75	9 719 376 896	22,74	24 675 685 440	23,73	62 292 331 392
24,72	156 254 486 400	25,71	389 861 188 608	26,70	968 881 334 400
27,69	2 401 604 036 480	28,68	5 943 999 466 080	29,67	14 718 828 604 800
30,66	36 489 120 287 104	31,65	90 531 973 320 960	32,64	224 302 545 792 990
33,63	552 555 915 961 088	34,62	1 345 521 360 969 600	35,61	3 216 056 123 389 440
36,60	7 490 278 550 241 824	37,59	16 869 275 678 196 480	38,58	36 469 040 038 061 376
39,57	75 117 167 475 907 200	40,56	146 393 515 772 750 496	41,55	268 119 161 284 331 136
42,54	458 751 110 448 999 360	43,53	729 280 862 203 782 144	44,52	1 072 405 790 365 371 360
45,51	1 453 109 164 616 688 384	46,50	1 809 232 996 157 293 440	47,49	2 065 243 290 390 040 320
48	2 158 800 489 098 126 488				

each n_e are listed in Table I. In a separate program each of these codes was expanded to find the partition function restricted to fixed n_e and n_o, the numbers of even- and odd-site flipped spins. The symmetry under the exchange of even and odd sites and $h_\pm$ provides a stringent test of the algorithm, which treats them in a very unsymmetric way. Setting $h_+=h_-=h$ or $y_+=y_-=y$ and collecting terms in Z for fixed $n=n_e+n_o$, one obtains the high-field polynomials, which are planned to be given and discussed in a separate paper. Their sum is the zero-field partition function, which is a 96th-order polynomial in u. It is given in tabular form in Table II.

III. ANALYSIS OF THE ZERO-FIELD PARTITION FUNCTION

Since Z is a polynomial in $u=e^{-4\beta}$, its analytic structure is trivial. It is completely described in terms of its zeros,

$$Z=2\prod_i (u-u_i)\ . \tag{3.1}$$

In the general case for a periodic cubic lattice of N sites there are $3N/2$ zeros. The free energy is then given by

$$-\beta F=N\left[\ln 2+\frac{1}{N}\sum_{i=1}^{3N/2}\ln(u-u_i)\right]\ . \tag{3.2}$$

We may express this as an integral over a real positive density function,

$$\rho(u)=\frac{1}{N}\sum_i \delta(u-u_i)\ . \tag{3.3}$$

Thus

$$-\beta F=N\left[\ln 2+\int du'\rho(u')\ln(u-u')\right]\ . \tag{3.4}$$

The internal energy has the even simpler form

$$U=-N\int du'\rho(u')/(u-u')\ . \tag{3.5}$$

In their celebrated discussion of the mathematical origin of phase transitions, Yang and Lee[6] argued that, when considered as an analytic function of the fugacity or activity, the partition function could be described in terms of the density of zeros in the complex plane, and that a phase transition is associated with this set of zeros approaching the real axis at the critical value. They also showed that under some restrictions, obeyed in the Ising model, the complex zeros of the partition function all lie on the unit circle in the activity (i.e., e^{-2h}) plane. Similar

reasoning, of course, applies to the complex temperature plane, though there is no circle theorem. To be precise, there is a distribution of zeros that at zero magnetic field and in the thermodynamic limit approaches arbitrarily close to the real axis at T_c. In the case of the two-dimensional Ising model, this distribution of zeros is known.[7] They all lie on a circle in the $\sinh(2\beta)$ plane, or on two circles in the $e^{-2\beta}$ plane. Also, these circles cross the real axis, for physical temperatures, just at T_c for the ferromagnetic and antiferromagnetic phase transitions. We might then expect that in the three-dimensional case as $N\to\infty$, (3.3) should give a well-defined limit for $\rho(u)$ with the zeros distributed on curves in the complex plane. Other types of behavior are possible, but this is the simplest. In this case, F and U are given by dispersion relations where one interprets $\rho(u)$ as a discontinuity across a branch cut. The placements of branch cuts are not unique in general, but if we require that the free energy of the finite lattice converge to an analytic function in the cut plane, then the choice is unique and dictated in terms of the zeros of Z.

In the finite-N case, the continuous distribution $\rho(u)$ is approximated by a discrete set of points. If ρ describes zeros on a curve, then in the finite-N case we may reasonably expect the zeros to lie on curves. This is certainly the case for the two-dimensional model where, for carefully chosen boundary conditions, the discrete zeros all lie exactly on the just mentioned circles. With this piece of intuition, we proceed to the partition function of the 4^3 system and compute the zeros. This is in principle perfectly straightforward, though I found it necessary to use double-precision arithmetic and some care in order to obtain the roots. There are some consistancy checks. First, the polynomial is real, so that all the roots that are complex should occur in pairs, and second, the polynomial is front-to-back symmetric so each root also occurs in a pair with its inverse. Both of these checks are satisfied to high precision. It is necessary to mention these things because it is not trivial to extract the roots of a 96th order polynomial whose coefficients range over 18 orders of magnitude.

The positions of the roots in the u plane are plotted in Fig. 1. The first and most striking impression is that the roots do have a strong tendency to lie on curves. A second glance reveals that the curves do approach the real axis at the known critical points $\beta_c=\pm 0.22$ for the ferromagnetic and antiferromagnetic transitions, which corresponds to $u=0.41$ and 2.43, respectively. Another interesting feature is a natural boundary which seems to isolate

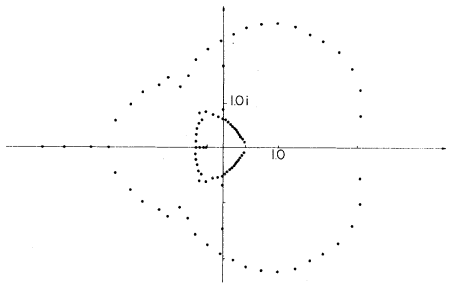

FIG. 1. 96 zeros of the partition function in the complex u plane.

the low-temperature point $u=0$, from the high-temperature limit at $u=1$. In previous analyses of low-temperature series,[8] one has observed and discussed the appearance of an unphysical singularity at negative real u. The series estimate for the singularity is $u=-0.2857$, which is reasonably well approximated by the first zero on the negative axis at $u=-0.307$. What is new is that the structure for negative u appears to be richer than imagined. Some hint of this structure is already seen in the $3\times3\times3$ case.[3]

The symmetry under $u\leftrightarrow 1/u$ can be exploited to map reciprocal pairs of zeros to the same point. This is the case if we choose

$$\sinh^{-2}(2\beta)=4u/(1-u)^2$$

as our variable. In Fig. 2 the 48 pairs of zeros are plotted. The structure around the unphysical singularity appears more concentrated while the zeros around the physical singularity are spread out. Although it is by no means certain, it is tempting to speculate that this "wishbone" structure will persist to the thermodynamic limit since it is very well defined for the 4^3 system. Also of some interest is the pattern of zeros when viewed in the standard high-temperature variable $\omega=\tanh\beta$. This is given in Figs. 3 and 4. The latter is an enlarged view of the region around the origin. The negative u axis is here mapped to the unit circle, and so the unphysical singularity and its associated branch cut appear as four short segments on the unit circle. It is an interesting question whether one may identify any stable complex singularities in the Padé analysis of high-temperature series, if indeed there are any, with structures in the 4^3 system.

IV. CONCLUSIONS

In this paper I have given an evaluation of the partition function of the three-dimensional Ising

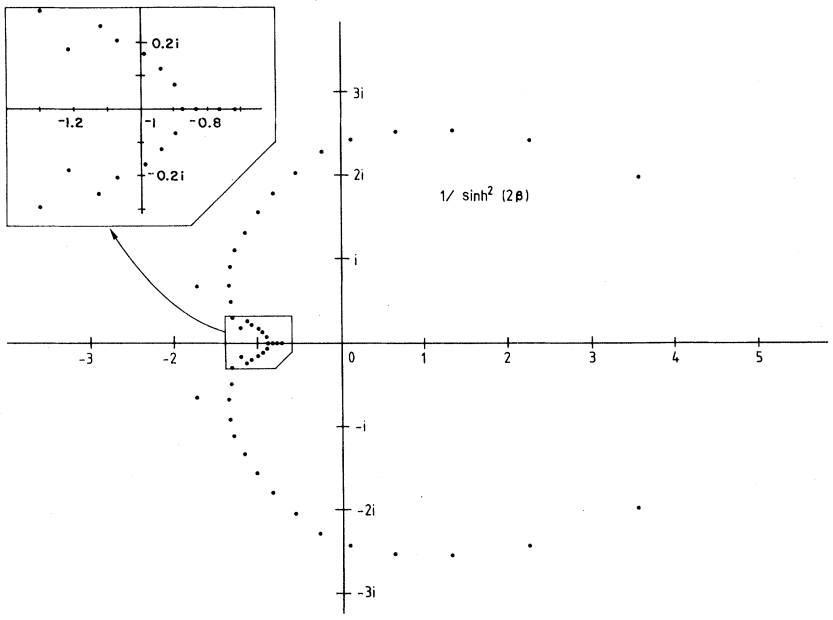

FIG. 2. Zeros of the partition function in the variable $\sinh^{-2}(2\beta)$.

model on a $4\times4\times4$ periodic lattice. The global analytic structure of the model appears faintly through the imperfect image of the zeros of the finite systems partition function. The main features that already have appeared in the $3\times3\times3$ case still exist and are somewhat more clear. In today's general emphasis on the universal aspects of critical behavior, there is not too much interest in the global analytic structure of models. I hope that these new results will help provide some insight into this problem.

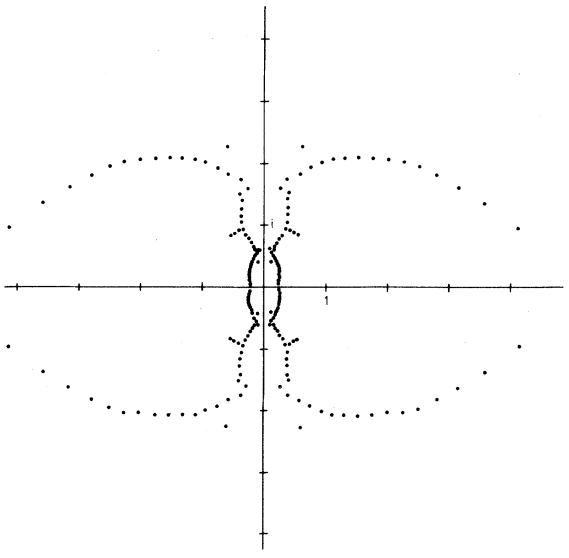

FIG. 3. Zeros of the partition function in the variable $\omega=\tanh\beta$.

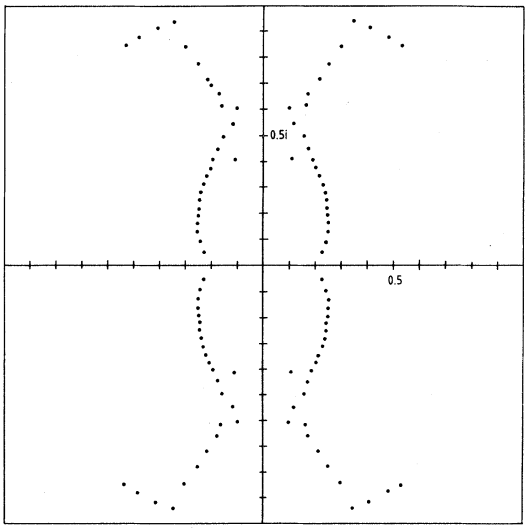

FIG. 4. Central portion of Fig. 3 enlarged.

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