Degeneracy of antiferromagnetic Ising lattices at critical magnetic field and zero temperature

B. D. Metcalf* and C. P. Yang
Department of Physics, The Ohio State University, Columbus, Ohio 43210
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The zero-point entropy and magnetization per site of the square and triangular Ising antiferromagnetic lattices in critical field have been calculated by a method that can be extended to three dimensions using a computer. The entropy for the triangular lattice is found to be $0.3333k \approx 1/3k$ per site.

I. INTRODUCTION

An appreciable fraction of the work on the Ising model has been devoted to antiferromagnetism. Various approximations have been applied to the model in order to obtain the magnetic phase diagram.[1-5] This diagram gives the critical temperature as a function of the applied magnetic field, and represents the line of singularities enclosing the region of antiferromagnetic ordering. Where this line intersects the field axis, the model gives different ground-state degeneracy depending on the topology of the lattice. For close-packed lattices, the ground state at $T=0$ and $B=0$ is degenerate. Wannier[6] computed the zero-point entropy for the triangular lattice which was later modified by Domb,[7] while Danielian[8-10] has shown that, despite the degeneracy of the antiferromagnetic fcc model, there is no zero-point entropy. The square and simple cubic lattices evidently do not have degeneracy at $T=0$ and $B=0$. It is the purpose of this paper to examine the ground-state degeneracy problem at the nonzero critical field for lattices of various geometry and dimension.

II. THE COUNTING PROBLEM

The energy of the antiferromagnetic Ising model of N spins in a magnetic field B is

$$E=-J\sum_{\langle ij\rangle}\sigma_i\sigma_j-B\sum_{i=1}^{N}\sigma_i\,, \tag{1}$$

where $J<0<B$. The magnetic moment is taken to be unity for each spin. $\sigma_i=\pm 1$ is the spin variable at the ith site and the first sum is over nearest-neighbor pairs of spins. The ground-state configuration when B dominates has all spins aligned with B and has an energy

$$E_0=-(\tfrac{1}{2}zJ+B)N\,,$$

where z is the number of nearest neighbors of each site. This state is nondegenerate. As B is reduced, a point is reached when overturning a number N_α of spins not neighboring one another will not change the energy E_0. Since $N_\alpha=\alpha N$ with $0<\alpha<1$, the entropy associated with this B is at least $N_\alpha k\ln 2$. This value of B is evidently $B_c=z|J|$. As B is further decreased, one enters the antiferromagnetic region. The counting problem associated with the entropy evaluation at B_c can be stated as follows: What is the allowed number of ways Ω_N of distributing spins antialigned to the field among N sites such that each such spin is surrounded completely by neighboring spins that are aligned?

III. BOUNDS AND INEQUALITIES FOR THE ENTROPY

(i) The entropy per site S is evidently bounded above by $k\ln 2$ for any lattice with N sites since $\Omega_N<2^N$. For loosely packed lattices (square, hexagonal, cubic, etc.), it is evident that $2^{N/2+1}-1<\Omega_N$, since half of the spins can be antialigned. This gives $\frac{1}{2}k\ln 2<S$. For triangular lattice, a little reflection shows $3\times 2^{N/3}-2<\Omega_N$. Thus, in general,

$$\alpha\ln 2<S/k<\ln 2\,, \tag{2}$$

where α is the maximum fraction of allowed antialigned spins on the lattice.

(ii) We next compare a square lattice and a triangular lattice with the same number of sites N. The triangular lattice can be regarded as a square lattice with diagonal bonds. Evidently, additional bonds serve to restrict the number of allowed configurations further. Thus,

$$\Omega_N(\text{square})>\Omega_N(\text{triangular})\,.$$

In general, the addition of bonds on a lattice will decrease the entropy. From this follows

$$\ln 2>S(\text{hexagonal})>S(\text{square})>S(\text{triangular})\,. \tag{3}$$

(iii) A cubic lattice of size $n\times n\times n$ can be regarded as n-plane-square lattices, each having a size $n\times n$ with additional bonding in the third direction. Patently we have,

$$[\Omega_{n\times n}(\text{square})]^n>\Omega_{n\times n\times n}(\text{cubic})\,,$$

hence we get,

$$S(\text{square}) > S(\text{cubic}).$$

It is then a simple matter to establish, using Eq. (2), that

$$S(\text{one dimensional}) > S(\text{hexagonal}) > S(\text{square}) > S(\text{cubic}) > S(\text{bcc}) \tag{4}$$

and

$$S(\text{triangular}) > S(\text{fcc}), \tag{5}$$

where a bcc lattice can be regarded as a collection of (110) planes.

IV. THE TRANSFER MATRIX

(i) Consider a one-dimensional system of m spins with periodic boundary conditions $(\sigma_{m+1} = \sigma_1)$ subject to the critical field constraint. We now define a transfer matrix as follows:

$$A_{\sigma_i \sigma_{i+1}} = \begin{cases} 1, & \text{if } \sigma_i \text{ and } \sigma_{i+1} \text{ are allowed in succession,} \\ 0, & \text{otherwise,} \end{cases} \tag{6}$$

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix},$$

The total number of allowed states is given by

$$\Omega_m = \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_m = \pm 1} A_{\sigma_1\sigma_2} A_{\sigma_2\sigma_3} \cdots A_{\sigma_m\sigma_1}$$

$$= \mathrm{Tr} A^m = \lambda_1^m + \lambda_2^m = [\tfrac{1}{2}(1+\sqrt{5})]^m + [\tfrac{1}{2}(1-\sqrt{5})]^m, \tag{7}$$

where λ_1 and λ_2 are the two eigenvalues of A. The entropy is readily found to be, as $m \to \infty$:

$$S = k \ln\tfrac{1}{2}(1+\sqrt{5}) = (0.4812\ldots)k. \tag{8}$$

The average magnetization is calculated from

$$\langle M \rangle_m = \frac{1}{\Omega_m} \sum_{\sigma_1} \cdots \sum_{\sigma_m} \sum_{i=1}^{m} \sigma_i A_{\sigma_1\sigma_2} \cdots A_{\sigma_m\sigma_1}, \tag{9}$$

where σ is the Pauli z-spin matrix. The evaluation of this is straightforward and yields

$$\lim_{m\to\infty} \frac{\langle M \rangle_m}{m} = \frac{1}{\sqrt{5}}, \tag{10}$$

which is well known.[11,12]

(ii) The above scheme can be extended to two-dimensional models. As an example, we carry out the formalism for the triangular lattice (square lattice with diagonal bonds) with periodic boundary conditions. Let the array be of m rows and n columns. The indexing of states is done column-wise by letting the state of the kth column be indexed by μ_k, $k = 1, 2, \ldots, n$. Each μ_k can take on Ω_m values since an allowed column state is an allowed state on a periodic chain of length m. The transfer matrix element $A\mu_i\mu_{i+1}$ is unity if column state μ_i can be followed by column state μ_{i+1} and is zero otherwise. The dimension of this matrix is evidently Ω_m. We call this matrix $A(\Omega_m)$. The total number of states allowed is

$$\Omega_{m\times n} = \mathrm{Tr}[A(\Omega_m)]^n. \tag{11}$$

The expression for the average magnetization is

$$\frac{\langle M \rangle}{mn} = \frac{1}{m\Omega_{mn}} \mathrm{Tr}\left[\begin{pmatrix} \gamma_1 & & & & 0 \\ & \gamma_2 & & & \\ & & \cdot & & \\ & & & \cdot & \\ 0 & & & & \gamma_{\Omega_m} \end{pmatrix} [A(\Omega_m)]^n \right], \tag{12}$$

where γ_i is the magnetization of a column in the state $\mu_k = i, i = 1, 2, \ldots, \Omega_m$. Whether the γ_i's take on values $m, m-2, m-4, \ldots$ down to 1 or 0 will depend on whether m is odd or even.

TABLE I. Average magnetization per spin for the triangular lattice critical field ground state with lattice width $m = 6$ and length n.

n	$\frac{\langle M \rangle}{N}$
2	0.661539
3	0.665072
4	0.678192
5	0.675231
6	0.674754
7	0.675052
8	0.675100
9	0.675029
10	0.675041
11	0.675054
12	0.675043
13	0.675048
14	0.675046
15	0.675047

TABLE II. Average magnetization per spin for increasing width m.

m	$\frac{\langle M \rangle}{N}$
2	0.6115
3	0.6667
4	0.6788
5	0.6745
6	0.6750
7	0.6752
8	0.6751
9	0.6751

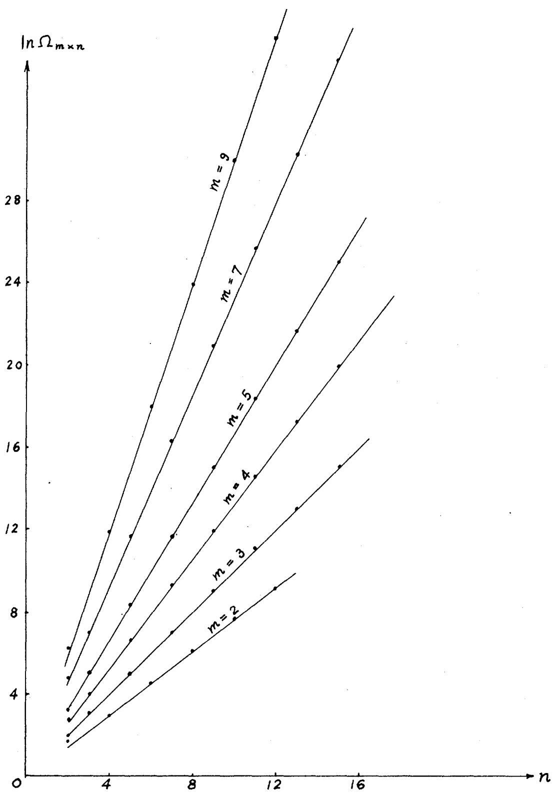

FIG. 1. Plot for $\ln\Omega_{mxn}=\ln \mathrm{Tr}[A(\Omega_m)]^n$ vs n for $m=2, 3, 4, 5, 7, 9$.

Since the size of the transfer matrix increases as $\Omega_m\times\Omega_m$, analytic solutions soon becomes unfeasible. For a lattice of $9\times n$ spins, there are 5776 matrix elements. We can, however, computerize the generation of the matrix elements by letting the computer select from the 2^m possible states only those Ω_m states satisfying the critical field requirement. Ω_m^2 comparisons are then made to obtain the matrix elements. From here, the S_{mn} and $\langle M\rangle/mn$ calculations can be carried out in a straightforward manner.

For each of the eight values of $m=2,3,\ldots,9$, S_{mn} and $\langle M\rangle/nm$ are evaluated for $n=2,3,\ldots,15$.

TABLE III. Results of linear data fit for $\ln \mathrm{Tr}\, A_m^n$ vs. n for $m=2,3,\ldots,9$, slope s_m and intercept b_m.

m	s_m/k	s_m/mk	b_m
2	0.7645	0.3823	0
3	1.005	0.3350	0
4	1.329	0.3323	0
5	1.667	0.3334	0
6	2.000	0.3333	0
7	2.333	0.3333	0
8	2.667	0.3333	0
9	3.000	0.3333	0

Table I shows the convergence of $\langle M\rangle/nm$ for $m=6$ to a value of 0.6750. Increasing m from 2 to 9 gives finally a value of

$$\langle M\rangle nm \rightarrow 0.6751 \tag{13}$$

for the magnetization of the triangular lattice (Table II). The computation of the entropy utilizes its extensive property. For sufficiently large mn, the total entropy should depend linearly on mn. Plot of $\ln \mathrm{Tr} A(\Omega_m)^n$ vs n is constructed for $n=2,\ldots,15$ and $m=2,3,\ldots,9$ (Fig. 1). Straight-line fits are made for each m using linear regression. The slopes $S_m=S_{mn}/n$ are given as a function of m for $m=2,3,\ldots,9$ (Table III). The entropy is then found to be

$$S=S_m/m=0.3333k\approx\tfrac{1}{3}k\,. \tag{14}$$

V. RESULTS AND DISCUSSIONS

Table IV contains the results of our calculations. The column labeled Monte Carlo corresponds to Monte Carlo (MC) calculations,[13-17] performed on lattices of size $N\gtrsim 3000$. We observe that except for the cubic entry the present calculations of magnetization agree with the MC calculations to well within five parts in 10^4. It is to be emphasized that since the Monte Carlo magnetization results join smoothly to the *finite temperature region*, the aforementioned agreement indicates strongly that the entropy associated with the

TABLE IV. Summarized results for various antiferromagnetic Ising models. Ground state in the critical magnetic field $B_c=z|J|$.

Lattice	$\left(\frac{\langle M\rangle}{N}\right)_{\text{Transfer matrix}}$	$\left(\frac{\langle M\rangle}{N}\right)_{\text{Monte Carlo}}$	$\frac{S}{Nk}$
One-dimensional ($z=2$)	0.4472	0.4475	0.4812
Square ($z=4$)	0.5470	0.5472	0.4075
Triangular ($z=6$)	0.6751	0.6753	0.3333
Simple cubic ($z=6$)	0.6208[a]	0.5902	0.3563[a]

[a] Results have only been carried as far as $3\times 4\times(n\rightarrow\infty)$.

ground-state degeneracy, which we calculated, is the same as the limit as $T \to 0^+$ of the finite temperature entropy.[18,19] The entropy calculations clearly satisfy the inequalities discussed in Sec. III. The triangular lattice, furthermore, gives an entropy value of $(0.3333\ldots)k$ which leads one to the conjecture that the exact value is $\frac{1}{3}k$. We can evidently extend this transfer matrix method to three-dimensional models. The indexing of states would be plane wise. The number of these plane states (and hence the dimension of the transfer matrix) increases so rapidly with the size of the plane that it is at the moment not quite economical to make extensive calculations on large lattices. As an example, computations for a simple cubic $3\times 4\times n$ lattice have been carried out and the magnetization is found to be 5% higher than the corresponding MC calculations. We expect, however, the rapid advance of computer hardware will soon make it feasible to treat three-dimensional systems.

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*Present address: MITRE Corp., P. O. Box 208, Bedford, Mass. 01730 Mail Stop B-130.

[1]A. Bienenstock, J. Appl. Phys. 37, 1459 (1966).
[2]D. M. Burley, Physica (Utr.) 27, 768 (1961).
[3]D. M. Burley, Proc. Phys. Soc. Lond. 85, 1163 (1965).
[4]C. Domb, Philos. Mag. (Suppl.) 9, 149 (1960).
[5]J. M. Ziman, Proc. Phys. Soc. Lond. A 64, 1108 (1951).
[6]G. H. Wannier, Phys. Rev. 79, 357 (1950).
[7]C. Domb, Adv. Phys. 9, 213 (1960).
[8]A. Danielian, Phys. Rev. Lett. 6, 670 (1961).
[9]A. Danielian, Physica (Utr.) 29, 67 (1963).
[10]A. Danielian, Phys. Rev. 133, A1344 (1964).
[11]K. Huang, *Statistical Mechanics* (Wiley, New York, 1965).
[12]M. Jaric and S. Milosevic, Phys. Lett. A 48, 367 (1974).
[13]B. D. Metcalf, Phys. Lett. A 45, 1 (1973).
[14]T. E. Shirley, Ph.D. thesis (The Ohio State University, 1972) (unpublished).
[15]B. D. Metcalf (unpublished).
[16]T. E. Shirley, Phys. Lett. A 42, 183 (1972).
[17]B. D. Metcalf and C. P. Yang (unpublished).
[18]R. B. Griffiths, J. Math. Phys. 6, 1447 (1965).
[19]H. S. Leff, Phys. Rev. A 2, 2368 (1970).