Two-Dimensional Ising Model in a Finite Magnetic Field*

Michael Plischke and Daniel Mattis
Belfer Graduate School of Science, Yeshiva University, New York, New York 10033
(Received 26 January 1970)

We present the results of numerical calculations giving accurate estimates of the magnetization of the two-dimensional Ising model on a square lattice. Moreover, we argue that these results are strict lower bounds to the correct magnetization $M(H, T)$. The estimates are obtained by dividing the infinite lattice into finite strips of width between two and nine spins and infinite length. The largest eigenvalue and the corresponding eigenvector of the transfer matrix are then obtained by an iterative process. The estimates of $M(H, T)$ converge to the correct answer for the infinite lattice everywhere except for a small region in the T-H plane. We also compute isotherms and critical isobar for the corresponding lattice gas. Finally, we propose a new approximation to the transfer matrix, exactly solvable in two dimensions for $H=O$, which reproduces exactly the critical-point behavior of the full Ising model.

The two-dimensional Ising model has never been solved in a finite field. The critical-point exponents,[1] however, have all been inferred from the exact solution of Onsager[2] in zero field or obtained from series expansion.[3] It remains to determine the magnetization $M(H,T)$ for finite H and $T \neq T_c$. Recently Mattis and Plischke[4] derived an analytic expression for a rigorous lower bound to $M(H,T)$ in terms of the zero-field internal energy $u\,(0,T)$ and the spontaneous magnetization $M(0,T)$. As the zero-field susceptibility could not be rigorously incorporated into this expression, the response to small fields was much too weak and the analytic bounds did not lie very close to the correct answer.

Another way of obtaining lower bounds to $M(H, T)$ is to divide the infinite lattice up into strips of infinite length and finite width. Since we have removed ferromagnetic bonds, the magnetization of each strip can only be lower than that of the infinite grid as has been shown by Griffiths.[5] The Kramers-Wannier transfer matrix for such a strip, N spins wide, is a $2^N \times 2^N$ matrix whose largest eigenvalue, and corresponding eigenvector, may be determined by a simple iterative process.[6]

The Hamiltonian for the ferromagnetic Ising model for an $M\times N$ lattice is

$$\mathcal{H} = -\tfrac{1}{2}\sum_{i=1}^{M}\sum_{j=1}^{N} J(\sigma_{i,j}\sigma_{i+1,j}+\sigma_{i,j}\sigma_{i,j+1}) - H\sum_{i,j}\sigma \ , \quad (1)$$

where $\sigma_i = \pm 1$. This has a critical temperature $kT_c = 2J/\ln(1+\sqrt{2}) \doteq 2.27J$ in the limit $M, N\to\infty$. The transfer matrix for a strip N spins wide is

$$\begin{aligned} V &= (V_2 V_3)^{1/2} V_1 (V_2 V_3)^{1/2} \ , \\ V_1 &= (2\sinh 2K)^{N/2}\exp\left(-K^* \sum_{j=1}^{N}\sigma_j^x\right) \ , \\ V_2 &= \exp\left(K\sum_{j=1}^{N}\sigma_j^z\sigma_{j+1}^z\right) \ , \\ V_3 &= \exp\left(\beta H\sum_{j=1}^{N}\sigma_j^z\right) \ , \end{aligned} \quad (2)$$

where $K = J/kT$, $K^* = -\frac{1}{2}\ln(\tanh K)$, and where we either leave free ends or wrap the strip on a torus in that $\sigma_{N+1}^z \equiv \sigma_1^z$. It may be argued that wrapping the strip on a torus restores some ferromagnetic bonds, so that the resulting curves may not be lower bounds. However, we have found that in all cases the magnetization of a toroidal strip monotonically increases as the strip gets larger so that we henceforth assume it to approach the correct answer from below. If the strip is M spins long, then as $M\to\infty$ the thermodynamics of the system are completely contained in the largest eigenvalue and the corresponding eigenvector of V. In particular, the free energy per spin is given by

$$f = F/MN = -(1/N)kT\ln\Lambda_{\max}(N, H, T) \ , \quad (3)$$

where $\Lambda_{\max}$ is the largest eigenvalue, and the magnetization is

$$m(H, T) = (1/N)M(H, T) = (1/N)\left\langle\psi_0\left|\sum_{j=1}^{N}\sigma_j^z\right|\psi_0\right\rangle, \quad (4)$$

where $|\psi_0\rangle$ is the largest eigenvector. The largest eigenvalue and its eigenvector are obtained by repeatedly multiplying V into a trial vector which must not be orthogonal to the largest eigenvector.[6] In a finite field this is achieved by taking as a starting point the state with all spins up. Error bounds can be computed by checking how close we are to an exact eigenstate of V, and by the increment in the results when an extra spin is added to the strip. Our present accuracy is sufficient for most practical purposes.

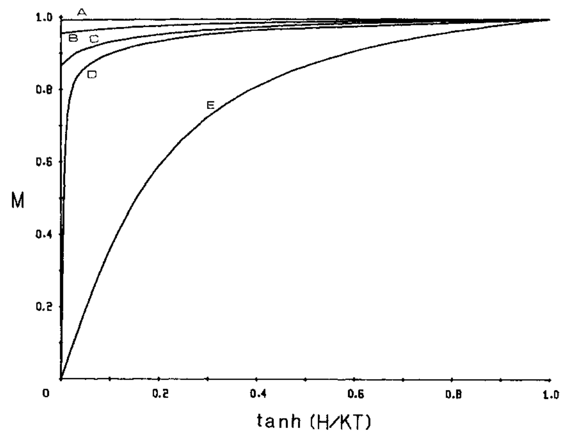

FIG. 1. Plot of $M(H, T)$ as function of $\tanh\beta H$ for various temperatures. (A) $T=0.61T_c$, $N=6$, (B) $T=0.8T_c$, $N=7$, (C) $T=0.927T_c$, $N=8$, (D) $T=T_c$, $N=9$, (E) $T=1.83T_c$, $N=6$. The critical behavior $m(H, T_c) = A(H/J)^{1/15}$ extends to $\tanh\beta H\approx 0.15$ in curve D.

We have carried out this procedure for strips up to nine spins wide and obtained the functions f and m. The magnetization is plotted for various fixed values of T against $\tanh\beta H$ in Fig. 1. In all cases the curves shown are lower bounds on $m(H, T)$ of the infinite Ising lattices. Except for $T = T_c$, $m(H, T)$ has converged to within 0.1% of the final answer at the value of N mentioned in the caption. Note that for $T < T_c$ the intercept with the M axis agrees accurately with the spontaneous magnetization $m(0, T)$ predicted by Onsager and calculated by Yang.[7,9] It is known that a strip of finite width cannot undergo a phase transition, and thus cannot have a spontaneous magnetization. The metastable nonzero spontaneous magnetization of our computer solution results because the solution was iterated only a finite number of times. A sufficiently large number of iterations ultimately decreases the magnetization to zero. However, our curves may be interpreted in a manner which guarantees a lower bound to $m(H, T)$. Since the zero-field magnetization of Yang, $m(0, T)$, is a *lower bound* to the spontaneous magnetization of the Ising model,[10] and since $m(H, T)$ is a concave function of H,[11] any straight line drawn between the point $m(0, T)$ and the nearest accurate value at another point $m(H_1, T)$, where $m(H_1, T)$ is moreover known to be a lower

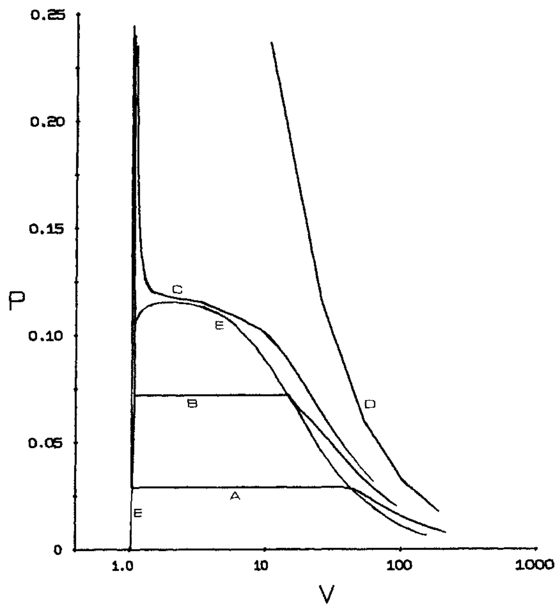

FIG. 2. Plot of isotherms for the lattice gas. (A) $T=0.8T_c$, (B) $T=0.927T_c$, (C) $T=T_c$, (D) $T=1.5T_c$. Curve (E) is the boundary of the two-phase region as determined from the analytic solution at $H=0$.

bound, will provide a lower bound to the magnetization over the entire range $0 \le H \le H_1$. Taking successively smaller values of H_1, one effectively generates the curves shown in Fig. 1 for $T < T_c$ as a lower bound to the exact result. At $T=T_c$, $m(H, T)$ has converged to within $\approx 0.1\%$ of the limit for all $H \ge 0.05J$ and to within 1% of the limit for $H \ge 0.1J$ for a strip nine spins wide. The critical region $m = A(H/J)^{1/15}$ behavior is indicated. The coefficient $A = 1.00 \pm 0.01$ for $J=1$. This was previously determined by Gaunt[3] to be 1.002, consistent with our result.

From the Ising model one can also obtain the thermodynamics of the classical lattice gas. The correspondence is[8]

$$P \leftrightarrow -(f+H+2J) , \qquad v \leftrightarrow 2/[1-m(H, T)] . \tag{5}$$

In the present paper we deal only with attractive forces $J>0$. We are presently studying the case of repulsive forces, where we find entirely different behavior. In Fig. 2 we show the isotherms of the lattice gas for some representative values of T. Again for $T \ne T_c$ the curves are accurate to $\approx 0.1\%$. At $T=T_c$ we plot the curve obtained from the nine-spin transfer matrix.

At high temperatures the isotherms approach those of the hard core, $J=0$, lattice gas given by

$$p/kT \equiv \ln[v/(v-1)] . \tag{6}$$

More detailed results such as table of values for the functions plotted in this paper will be included in a thesis to be submitted to Yeshiva University by one of us (M. P.) and will be made available upon request.

While all the above work was performed on the exact transfer matrix, we would like to call attention to an approximation of the transfer matrix which greatly simplifies this type of numerical calculation. If one combines the exponents in the V's, neglecting Baker-Hausdorff corrections,

$$V \approx (2 \sinh 2K)^{N/2}$$

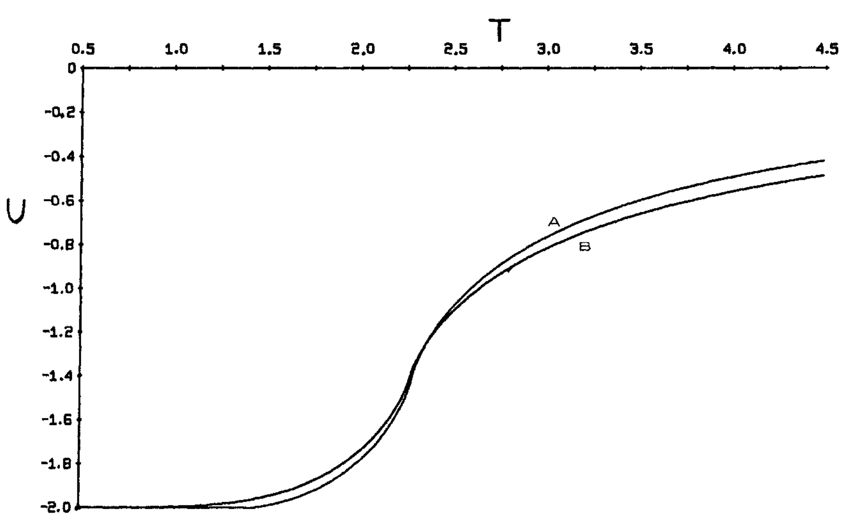

FIG. 3. Plot of internal energies of the pseudomodel and the Ising model in zero field as function of temperature. (A) $U_P(0, T)$; (B) $U_I(0, T)$. The deviation from infinite slope at T_c results from inertia in the mechanical plotter, not from any significant computer error.

$$\times \exp\left[K\sum_{j=1}^{N}\sigma_j^z\sigma_{j+1}^z - K^*\sum_{j=1}^{N}\sigma_j^x + \beta H\sum_{j=1}^{N}\sigma_j^z\right], \tag{7}$$

then at $H=0$ one can calculate the thermodynamic properties of this "pseudo-transfer-matrix" using the same methods as for the full Ising model.[9] Surprisingly, one obtains precisely the same critical properties:

$$\begin{aligned} &T_p = T_c \ , \\ &U_p(0, T_c) = U_I(0, T_c) \ , \\ &M_p(0, T) \sim |T - T_c|^{1/8} \ , \\ &C_p(0, T) \sim \ln|T - T_c| \ , \end{aligned} \tag{8}$$

where T_p is the transition temperature of the pseudomodel and U_p, M_p, C_p are the internal energy, spontaneous magnetization, and specific heat of the pseudomodel. The exact zero-field internal energy of this pseudomodel is plotted in Fig. 3 along with the exact internal energy of the complete Ising model as a function of temperature. The usefulness of this approximation is that one need only obtain the largest eigenvalue and eigenvector of the matrix in the exponent. This matrix is sparse, i.e., has a *large* number of zeros, so that transfer matrices with more spins may be treated. We plan to make use of this important property in several future calculations.

We would like to thank Professor L. F. Landovitz and Dr. W. Langer for stimulating discussions.

---

*Research supported in part by Grant No. AF-69-1642.

[1]See, for example, L. P. Kadanoff *et al.*, Rev. Mod. Phys. 39, 395 (1967); M. E. Fisher, Rept. Progr. Phys. 30, 615 (1967).

[2]L. Onsager Phys. Rev. 65, 117 (1944).

[3]D. S. Gaunt, Proc. Phys. Soc. (London) 92, 150 (1967).

[4]Daniel C. Mattis and Michael Plischke, J. Math. Phys. 10, 1107 (1969).

[5]R. B. Griffiths, J. Math. Phys. 8, 478 (1967).

[6]A. S. Householder, *Principles of Numerical Analysis* (McGraw-Hill, New York, 1953), p. 150 ff.

[7]C. N. Yang, Phys. Rev. 85, 808 (1952).

[8]K. Huang, *Statistical Mechanics* (Wiley, New York, 1963), p. 334. The properties of the lattice gas were evaluated in this book, using relatively crude molecular-field theory. We should also note early, accurate results in lattice gases, particularly for $J<0$, the numerical work by L. K. Runnels [Phys. Rev. Letters 15, 581 (1965)] on the "hard square" lattice gas (the $J\to-\infty$ limit of the present model), and the related work of A. Bellemans, in *Statistical Mechanics*, edited by T. Bak (Benjamin, New York, 1967), p. 373, are to be noted.

[9]T. D. Schultz, D. C. Mattis, and E. H. Lieb, Rev. Mod. Phys. 36, 856 (1964).

[10]R. B. Griffiths, Phys. Rev. 152, 240 (1966).

[11]R. B. Griffiths, C. A. Hurst, and S. Sherman, J. Math. Phys. 11, 790 (1970).