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Three-Spin Interaction Ising Model with a Nondegenerate Ground State at Zero Applied Field

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The field–temperature phase diagram of a two-dimensional, three-spin interaction Ising model is studied using two different methods: mean field approximation and numerical transfer matrix techniques. The former leads to a rather rich phase diagram in which two separate phases with different symmetries can be found, and which presents first-order transition lines, a triple point, and a critical end point, like the solid–liquid–gas phase diagram of a pure compound. The numerical transfer matrix study confirms part of these results, but does not clearly evidence the existence of the less symmetric phase.

KEY WORDS: Ising spins; finite-width strips; first-order phase transition.

1. INTRODUCTION

Although three-spin interactions (and, more generally, interactions involving "products" of an odd number of spins) cannot be taken into account for systems invariant under time reversal, they are allowed to appear when this constraint is removed, as in the lattice-gas representation of fluids with three-body interactions,[1,2] and in the Ising spin description of a certain class of cellular automata (Domany–Kinzel[3]). Our purpose is not to discuss the relevance of three-spin interactions in real systems, but to understand from a theoretical point of view the role played by such interactions in the occurrence of phase transitions.[4]

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[4] Following the solution of the eight-vertex model by Baxter, increasing interest was devoted to three-spin Ising models. We cannot quote this work extensively here; significant contributions can be found in Refs. 4–7.

In this paper, our aim is to study the two-dimensional system described by the Hamiltonian

$$\mathscr{H} = -J \sum_{\langle i,j,k \rangle} \sigma_i \sigma_j \sigma_k - H \sum_i \sigma_i \tag{1}$$

where the spins $\sigma_i = \pm 1$ are located at the vertices of a square lattice, and the first sum in the rhs of (1) runs over all triplets such that sites i, j, k belong to the same elementary square (Fig. 1a). If $J > 0$, then for $H = 0$ the minimum of $\mathscr{H}$ is obviously obtained when and only when all spin variables are equal to one.

With a suitable choice of the lattice and the triplets involved in the interactions, many other models sharing the same property could be defined. Examples of such systems are shown in Figs. 1b–1d. For each of these models, the complete lattice can be generated by the Bravais translations of an elementary cell defined by the interactions. Only the point group of the elementary cell and the group of the translations that generate the Bravais lattice leave the Hamiltonian invariant: therefore, the possible order parameters of the system, if any, should necessarily be associated with the breaking of one of these symmetries.

To our knowledge, there exists no exact solution for any of these models even at zero applied field. Therefore, in the absence of exact results, we will use general arguments and rely on the convergence of the conclusions obtained by various approximate methods. Our aim in this paper is to show that such systems do exhibit a variety of phase transitions.

We shall focus now on the square lattice model as a typical example. Due to the remarkable feature that its ground state at zero applied field is nondegenerate, the system does not exhibit a symmetry-breaking order parameter, and the only possible phase transition (at zero field), if any, should be associated with a discontinuity of the magnetization. However, we shall see that the magnetization per spin, which is equal to 1 at $T = 0$, remains strictly positive at any finite temperature as a consequence of a Griffiths inequaltiy which rules out the existence of a paramagnetic phase. On the other hand, if we want to break the translational invariance of the system and try to exhibit the corresponding phase transition, it is necessary to apply an external field in order to reverse some of the spins and find a degenerate ground state.

In what follows we shall first determine the ground states of the system in the presence of an external uniform magnetic field and find that, as a function of the field, the system undergoes two first-order transitions. We shall then study the system at finite temperature within a mean field approximation in which the form of the trial Hamiltonian reflects the structure of the ground states, and determine the corresponding field–

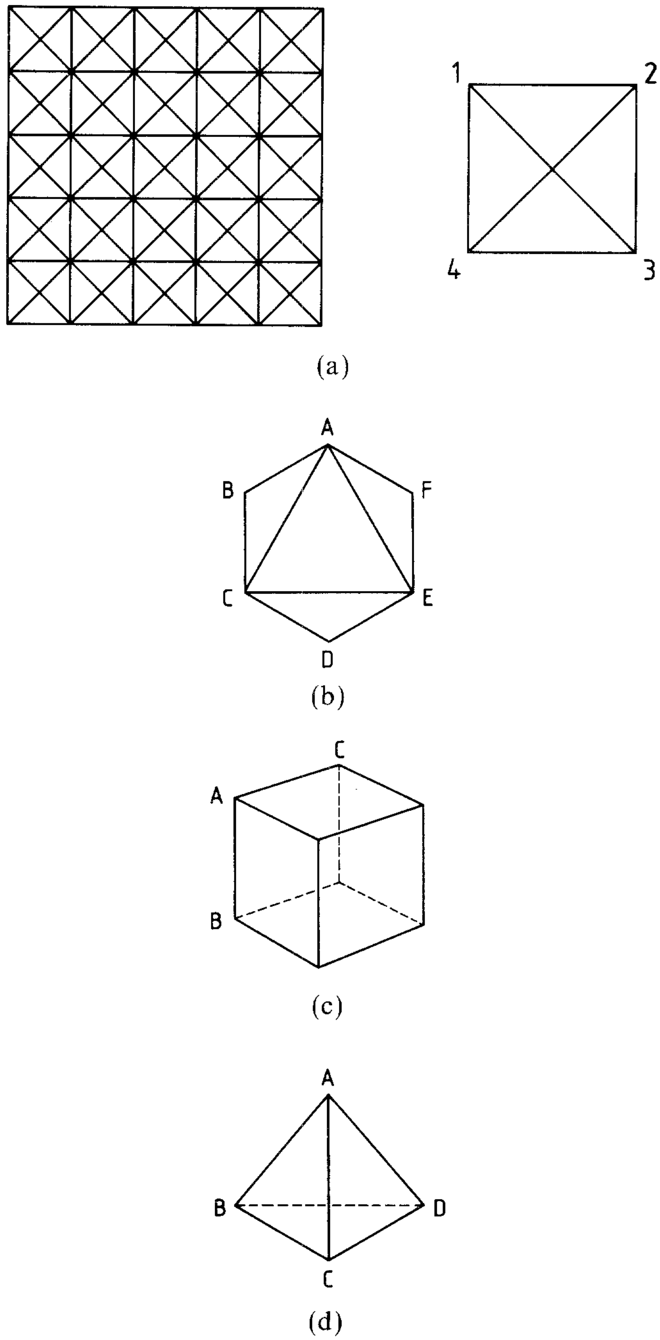


Fig. 1. (a) Two-dimensional square lattice and the corresponding unit cell. (b) Two-dimensional triangular hexagonal lattice, interacting triplets: *ABC*, *CDE*, *EFA*, and *ACE*. (c) Three-dimensional cubic lattice; interacting triplets: all those obtained from *ABC* by the point group symmetry of the cube. (d) Spinel lattice; interacting triplets: *ABC*, *BCD*, *ACD*, and *ABD*.

temperature phase diagram. As a more precise and confirming approach to these results, in a subsequent section, we shall present the conclusions obtained from the transfer matrix technique applied to finite-width systems.

2. MEAN FIELD APPROXIMATION

As a first step, we determine the ground states of the square lattice in the presence of a uniform applied field. The Hamiltonian (1) can be written in the equivalent form

$$\mathscr{H} = \sum_{\text{sq}} -J(\sigma_1\sigma_2\sigma_3 + \sigma_2\sigma_3\sigma_4 + \sigma_3\sigma_4\sigma_1 + \sigma_4\sigma_1\sigma_2) - \tfrac{1}{4}H(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4) \tag{2}$$

Here, the four spins σ_1, σ_2, σ_3, σ_4 belong to the same elementary square: the summation now runs over all squares of the lattice, and the 1/4 factor before H takes into account the fact that each spin belongs to four squares.

We now look for the configurations of four spins that minimize the energy of one elementary square. If the respective configurations in adjacent squares allow for a complete tiling over the whole lattice, then the minimum of $\mathscr{H}$ will be obtained as the sum of the minima of each of its terms. It is easy to see that

$$\begin{aligned} &-J(\sigma_1\sigma_2\sigma_3 + \sigma_2\sigma_3\sigma_4 + \sigma_3\sigma_4\sigma_1 + \sigma_4\sigma_1\sigma_2) - \tfrac{1}{4}H(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4) \\ &\quad = -\tfrac{2}{3}Jm(16m^2 - 10) - Hm \end{aligned} \tag{3}$$

where $m = (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)/4$ can take the five values -1, $-1/2$, 0, 1/2, 1.

The corresponding five energies as functions of H are represented in Fig. 2. Their comparison shows that the various ground states for an elementary square are:

(a) if $-\frac{4}{3}J \leqslant H$, $\quad m = +1$ (4 spins up)

(b) if $-12J \leqslant H \leqslant -\frac{4}{3}J$, $\quad m = -\frac{1}{2}$ (1 spin up, 3 down)

(c) if $H \leqslant -12J$, $\quad m = -1$ (4 spins down)

In each case, compatibility over the whole lattice is ensured. The state $m = -\frac{1}{2}$ corresponds to a structure in which the unit cell is a square built with four elementary squares (Fig. 3a), but this structure is generally not periodic (Fig. 3b) and highly degenerate, although its entropy per spin goes to zero as $1/\sqrt{N}$, where N is the number of spins.

The stability conditions (a)–(c) show that, at $T = 0$, when H varies, the system undergoes two first-order phase transitions at $H_{c_2} = -12J$ and $H_{c_1} = -\frac{4}{3}J$, respectively.

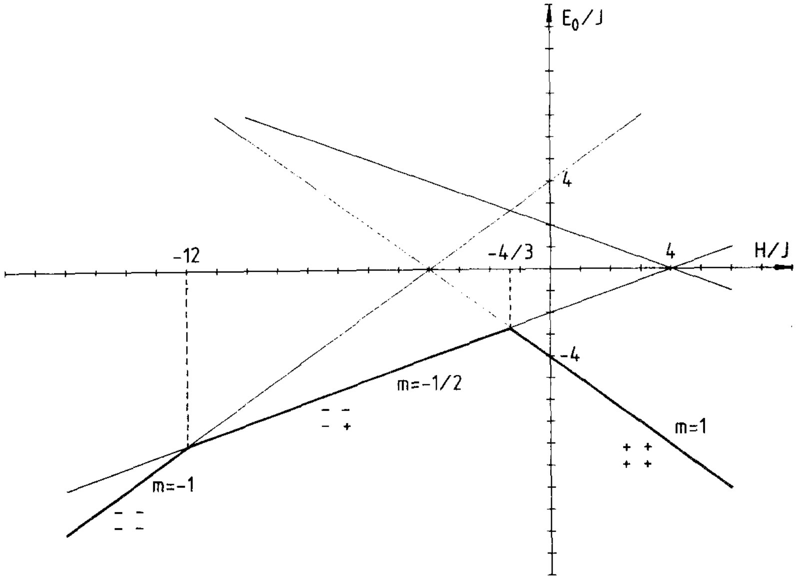


Fig. 2. Energy per elementary square as a function of the applied field for all the possible spin configurations.

−	−	−
−	+	−
−	−	−

a

−	−	−	+	−	+	−	−	−
−	+	−	−	−	−	−	+	−
−	−	−	+	−	+	−	−	−
−	+	−	−	−	−	−	+	−
−	−	−	+	−	+	−	−	−
−	+	−	−	−	−	−	+	−
−	−	−	+	−	+	−	−	−
−	+	−	−	−	−	−	+	−
−	−	−	+	−	+	−	−	−
−	+	−	−	−	−	−	+	−
−	−	−	+	−	+	−	−	−
−	+	−	−	−	−	−	+	−
−	−	−	+	−	+	−	−	−

b

Fig. 3. (a) Unit cell corresponding to the state $m = -\frac{1}{2}$. (b) Example of a nonperiodic structure obtained by tiling unit cells of type *a*.

Note that precisely at $H=H_{c_2}$ a peculiar situation occurs. Any spin configuration for which any two up spins cannot be at a distance less than two lattice spacings is a ground state. In other words, the up spins can be considered as a lattice gas of particles with a variable density and a hard-core repulsion. The number of corresponding configurations can easily be shown to be larger than $2^{N/4}$, so that a large residual entropy per spin ($S_0 \geqslant 0.1733$) is observed at $T=0$, $H=H_{c_2}$. The situation at $H=H_{c_1}$ is completely different, due to the fact that elementary squares with $m=1$ and elementary squares with $m=-\frac{1}{2}$ cannot coexist: thus, at $H=H_{c_1}$ the allowed ground states are all those found for $m=-\frac{1}{2}$, plus the state with all spins up.

Although our study will be limited to the two-dimensional lattice, the previous minimization procedure can be extended to a d-dimensional hypercubic lattice. For $d=3$ (Fig. 1c) there are six elementary squares per cube: at $T=0$, when H varies there are still two first-order transitions characterized by the same magnetization jumps as for $d=2$. The $m=-\frac{1}{2}$ solution is now found to be stable within the domain $-36J \leqslant H \leqslant -4J$ and the corresponding structure is strictly periodic, the up spins being located at the sites of a body-centered cubic lattice with a unit cell containing eight elementary cubes. At $H=-36J$, each of these up spins can now be either up or down, so that at this point the ground state is again highly degenerate, with a finite entropy $S_0=\frac{1}{4}\ln 2$ per spin (the lattice gas description used in the two-dimensional case remains valid).

For $d=4$ there are 24 two-dimensional square facettes per cube, and in this case we have not been able to satisfy the compatibility conditions between facettes for the $m=-\frac{1}{2}$ solution. However, the first-order phase transition where the mean magnetization per spin jumps from 1 to $-1/2$ does exist for $d=\infty$ (constant interaction model[8]), although there is no sublattice description of the $m=-1/2$ phase, i.e., no breaking of the translational symmetry is available in this case.

The structure of the ground states as a function of H leads us to assume that, at nonzero temperature, the state of the system can be characterized by two parameters m_1 and m_2 which are the respective magnetizations per spin of two subclasses of the N spins, such that at $T=0$ we have the following equivalences:

$$m=1 \Leftrightarrow m_1=1 \text{ and } m_2=1$$

$$m=-\tfrac{1}{2} \Leftrightarrow m_1=1 \text{ and } m_2=-1$$

$$m=-1 \Leftrightarrow m_1=-1 \text{ and } m_2=-1$$

Subclasses 1 and 2 contain, respectively, $N/4$ and $3N/4$ spins. In two dimensions, these subclasses do not in general form sublattices, due to the nonperiodic structure of the phase $m = -\frac{1}{2}$, while at $d = 3$ the spins belonging to subclass 1 are located at the sites of the bcc lattice mentioned above.

As a consequence of the previous remarks, in order to determine the variational free energy of the system, we choose a trial Hamiltonian $\mathscr{H}_0$ of the form

$$\mathscr{H}_0 = -h_1 \sum_{i \in \{1\}} \sigma_i - h_2 \sum_{j \in \{2\}} \sigma_j \tag{4}$$

where $\{1\}$ and $\{2\}$ denote, respectively, the subclasses 1 and 2. In each elementary square, there is exactly one spin belonging to $\{1\}$ and three spins belonging to $\{2\}$. Therefore, out of the four corresponding interacting triplets, one contains exclusively spins of subclass 2; each of the other three contains one spin of subclass 1 and two spins of subclass 2.

It is straightforward to write down the variational free energy per spin:

$$\begin{aligned}\frac{F}{N} = &-\frac{1}{4\beta}\ln(2\cosh\beta h_1) - \frac{3}{4\beta}\ln(2\cosh\beta h_2)\\ &-\frac{1}{4}h_1 m_1 - \frac{3}{4}h_2 m_2 - 3Jm_1 m_2^2 - Jm_2^3 - \frac{1}{4}Hm_1 - \frac{3}{4}Hm_2\end{aligned} \tag{5}$$

where

$$m_i = \tanh\beta h_i \qquad (i = 1, 2) \tag{6}$$

Minimizing with respect to the variational parameters h_1 and h_2, we obtain the equations

$$h_1 = 12Jm_2^2 + H \tag{7a}$$

$$h_2 = 8Jm_1 m_2 + 4Jm_2^2 + H \tag{7b}$$

so that, taking (6) into account,

$$m_1 = \tanh\beta(12Jm_2^2 + H) \tag{8a}$$

$$m_2 = \tanh\beta(8Jm_1 m_2 + 4Jm_2^2 + H) \tag{8b}$$

These equations have an obvious solution $m_1 = m_2 = m$ provided

$$m = \tanh\beta(12Jm^2 + H) \tag{9}$$

yields the minimum value of (5). A simple graphical inspection (Fig. 4) shows that for given field and temperature, (9) has one or three solutions; the latter case corresponds to the existence of two minima for the free

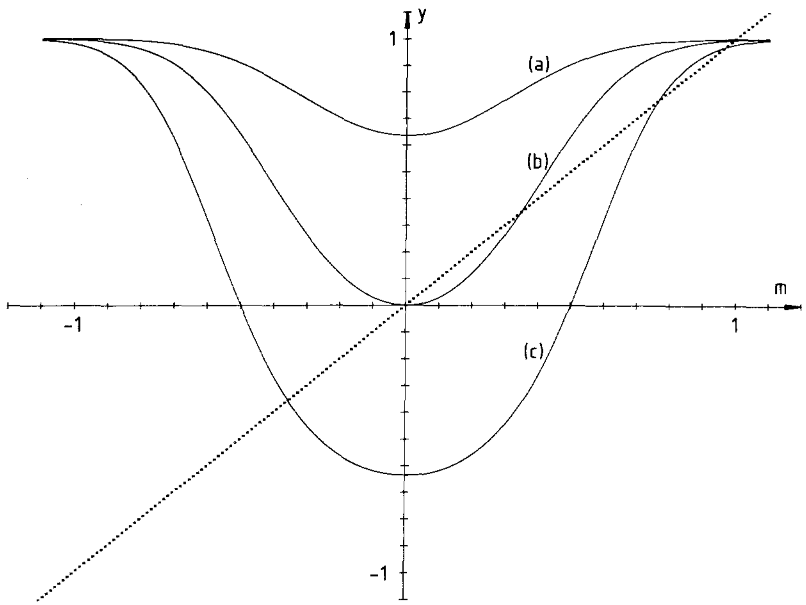


Fig. 4. Graphical solution of Eq. (9) for three typical plots of $y = \tanh \beta(12Jm^2 + H)$. (a) $\beta J = 0.25$; $H/J = 3$. (b) $\beta J = 0.25$; $H/J = 0$. (c) $\beta J = 0.25$; $H/J = -3$.

energy and the possible occurrence of a first-order transition characterized by a discontinuous magnetization. Such a transition is not characterized by a symmetry-breaking order parameter.

In the contrary, solutions of (8a) and (8b) with $m_1 \neq m_2$ if any correspond to a breaking of the translational invariance of the system and in this case $m_1 - m_2$ will be a suitable order parameter.

We have solved (8a) and (8b) in the following manner: m_1 in the rhs of (8b) is replaced by its expression as a function of m_2 given by (8a), yielding

$$m_2 = \tanh\{\beta[8Jm_2 \tanh \beta(12Jm_2^2 + H) + 4Jm_2^2 + H]\} \tag{8c}$$

For a given temperature and field, the possible solutions m_2 of (8c) are found numerically. Each of them corresponds to well-defined values of m_1, h_1, and h_2, which, after being replaced into (5), determine the most stable solution.

We have thus been able to determine the complete field–temperature phase diagram, which is represented Fig. 5 and has the following salient features.

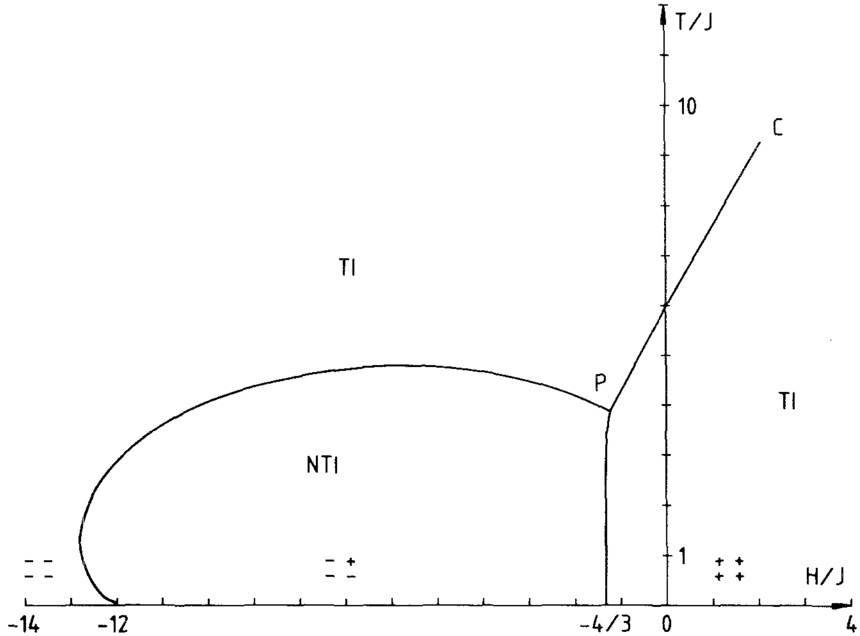


Fig. 5. Field–temperature phase diagram of the two-dimensional square model within the mean field approximation.

All phase transitions are first order. A non-translational-invariant (NTI) phase, characterized by a nonzero value of the order parameter $m_1 - m_2$, is stable in a finite domain. The translational-invariant (TI) phase is stable everywhere else; this phase is characterized by $m_1 = m_2 = m$; this parameter is discontinuous along a liquid–gas type line, which ends at a critical point whose coordinates are $H_c/J = 2.083$, $T_c/J = 9.238$. The location of this critical point can be determined analytically as follows: if $m = y(m, T, H)$ is the self-consistent equation governing the behavior of m, the critical point is determined by expressing that the equation $y(m, T, H) - m = 0$ has a triple root m_c in m, which implies

$$\begin{aligned} &y(m_c, T_c, H_c) = m_c \\ &\frac{\partial y}{\partial m}(m_c, T_c, H_c) = 1 \\ &\frac{\partial^2 y}{\partial m^2}(m_c, T_c, H_c) = 0 \end{aligned} \tag{10}$$

Here $y(m, T, H) = \tanh(12Jm^2 + H)/T$ and (10) is found to have the solution

$$m_c = \frac{1}{\sqrt{3}}, \qquad \frac{T_c}{J} = \frac{16}{\sqrt{3}}, \qquad \frac{H_c}{J} = \frac{8}{\sqrt{3}} \ln(2 + \sqrt{3}) - 4 \tag{11}$$

It is worth mentioning that the NTI–TI first-order transition line exhibits a point where $dT/dH = 0$, which implies as a consequence of the Clausius–Clapeyron equation that at this point the magnetization jump is zero, and another point where $dT/dH = \infty$, which implies that the entropy jump at this point is zero. The phase diagram also exhibits a triple point P whose coordinates, determined numerically, are

$$H_P/J \cong -1.25, \qquad T_P/J \cong 3.88$$

Qualitatively, the phase diagram shows a striking similarity with the pressure–temperature diagram of a pure compound. Both of them exhibit a triple point and a critical point. The fluid phase is the equivalent of our TI phase and the role of the crystalline phase is played by our NTI phase. Just as the crystalline phase breaks the infinitesimal translational invariance of the fluid phase, the NTI phase breaks the translational invariance the TI phase lattice.

When solving the self-consistent equations that determine m_1 and m_2, we did not have to pay special attention to the particular value $H = 0$. In this case, as the temperature increases the system exhibits at $T/J = 5.95$ a first-order phase transition where the magnetization drops from a positive finite value to zero. However, the existence of this high-temperature, zero-field "paramagnetic" phase is disproved by an inequality due to Griffiths,[9] which states that, given two sets of spins Ω_1 and Ω_2 such that $\Omega_1 \subset \Omega_2$, then if $S_i \in \Omega_1$, the thermal average of S_i performed over the states of Ω_1 is smaller than that performed over the states of Ω_2; choosing now Ω_1 as four spins at the vertices of an elementary square and Ω_2 as the whole set of the N spins, we find easily that, at zero applied field,

$$\langle S_1 \rangle_{\Omega_1} = \langle S_1 \rangle_{\text{square}} = (\tanh \beta J)^3$$

$$\langle S_1 \rangle_{\Omega_2} = m \qquad \text{in the TI phase}$$

Thus, one must have

$$m \geqslant (\tanh \beta J)^3 \tag{12}$$

The violation of this inequality by the mean field results at zero field is not too surprising, since mean field predictions are exact for an infinite-dimensional model, or, equivalently, for a constant interaction model where the interaction has to be renormalized, changing J into J/N^2 for a three-spin interaction; in the thermodynamic limit, (12) becomes $m \geqslant 0$, in agreement with our results.

As a final remark to this section, we underline the fact that an identical phase diagram would be obtained for the three-dimensional case after rescaling H, the NTI phase being in this case periodic and $m_1 - m_2$ becoming a real order parameter.

Predictions of the mean field theory are known to be sometimes questionable, but often qualitatively correct. In the next section we shall try to confirm or disprove the existence and order of the phase transitions that have just been found, using a completely different technique in which the two-dimensional character of the system is correctly taken into account.

3. TRANSFER MATRIX APPLIED TO FINITE-WIDTH SYSTEMS

3.1. General Outline

In this section we present some results obtained from the numerical study of strips of finite width n (vertical direction) and very large length L (horizontal direction) as shown in Fig. 6. Each site of the square lattice is now characterized by two indices (i, j) and we shall assume cyclic boundary conditions in both directions so that

$$\left.\begin{array}{ll} \text{for any } i, & \sigma_{i,j} = \sigma_{i,j+n} \\ \text{for any } j, & \sigma_{i+L,j} = \sigma_{i,j} \end{array}\right\} \quad i = 1,..., L, \quad j = 1,..., n$$

We can write the Hamiltonian of this system as

$$\mathscr{H}_{n,L} = \sum_{i=1}^{L} \mathscr{H}_{i,n}$$

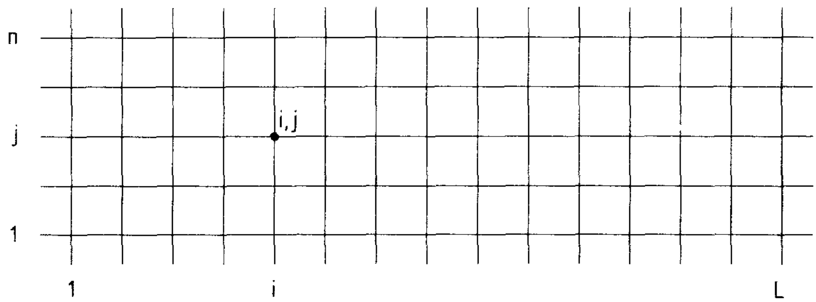


Fig. 6. Strip of width n and length L.

with

$$\mathscr{H}_{i,n} = \sum_{j=1}^{n} -J(\sigma_{i,j}\sigma_{i,j+1}\sigma_{i+1,j+1} + \sigma_{i,j+1}\sigma_{i+1,j+1}\sigma_{i+1,j} + \sigma_{i+1,j+1}\sigma_{i+1,j}\sigma_{i,j} + \sigma_{i+1,j}\sigma_{i,j}\sigma_{i,j+1}) - \tfrac{1}{2}H(\sigma_{i,j} + \sigma_{i+1,j})$$

Each vertical row of spins, characterized by index i, has 2^n possible configurations. Given two respective configurations C_k and C_l of the two neighboring columns labeled by i and $i+1$, let $E(C_k, C_l)$ be the corresponding value of $\mathscr{H}_{i,n}$. If we now construct the $(2^n \times 2^n)$ symmetric matrix $\mathscr{M}$ whose the elements are given by

$$\mathscr{M}_{k,l} = \exp[-\beta E(C_k, C_l)] \tag{13}$$

then the well-known transfer matrix formalism ensures that the free energy per spin of the strip, in the limit where its length L goes to infinity, is given by

$$f_n(\beta, J, H) = -\frac{1}{n\beta} \ln[\lambda_{n,\max}(\beta, J, H)] \tag{14}$$

where $\lambda_{n,\max}$ is the largest (positive) eigenvalue of $\mathscr{M}$ at given values of n, β, J, H.

Therefore it is possible, in principle, to extract all the thermodynamic quantities of interest for any system of finite width n and infinite length. Following the evolution, for increasing values of n, of quantities that may display a "critical" behavior in the $n \mapsto \infty$ limit is an essential approach to the properties of the real, two-dimensional system. Sophisticated numerical methods of investigation of these limiting properties are available in the case of critical phenomena associated with second-order phase transitions (e.g., Ref. 10).

Our situation here is peculiar in the sense that we have to cross-check mean field predictions that involve only first-order phase transitions. Therefore, what we have done was essentially to determine the following quantities: magnetization/spin

$$m_n(\beta, J, H) = -\frac{\partial}{\partial H} f_n(\beta, J, H)$$

susceptibility/spin

$$\chi_n(\beta, J, H) = -\frac{\partial^2}{\partial H^2} f_n(\beta, J, H)$$

internal energy/spin

$$U_n(\beta, J, H) = \frac{\partial}{\partial\beta}[\beta f_n(\beta, J, H)]$$

entropy/spin

$$S_n(\beta, J, H) = \beta^2 \frac{\partial}{\partial\beta} f_n(\beta, J, H)$$

specific heat/spin

$$C_n(\beta, J, H) = -\beta^2 \frac{\partial^2}{\partial\beta^2}[\beta f_n(\beta, J, H)]$$

For a given value of n one can obtain numerically the variation of these quantities at fixed temperature as H varies and study their evolution as n is increased.

We now wish to make precise the conditions under which our numerical tasks have been carried out, and also (in part as a direct consequence of these conditions) the limitations to our subsequent conclusions:

1. The widths considered for the strips lie in the range $n = 2$–6.

2. For each value of n, the largest eigenvalue of the transfer matrix $\mathscr{M}$ at fixed β, J, H has been obtained by an iterative process: starting with some initial normalized vector V_0 with positive components, we obtain

$$\begin{aligned} \mathscr{M} V_0 &= W_1, & W_1/\|W_1\| &= V_1 \\ \mathscr{M} V_1 &= W_2, & W_2/\|W_2\| &= V_2, \text{ etc.} \\ \mathscr{M} V_{l-1} &= W_l, & W_l/\|W_l\| &= V_l, \text{ etc.} \end{aligned}$$

when l goes to infinity; then

$$\|W_l\| \mapsto \lambda_{n,\max}(\beta, J, H)$$

and V_l converges toward the corresponding eigenvector. The iterative process was stopped as soon as

$$\sup\left(\left|\frac{\|W_l\| - \|W_{l-1}\|}{\|W_{l-1}\|}\right|, \|V_l - V_{l-1}\|\right) < 10^{-11}$$

3. Guided by the results of some preliminary trials and by the mean field predictions, our investigations in the (H, T) plane have taken place in

the domain $-14 \leqslant H/J \leqslant 2$, $0 \leqslant T/J \leqslant 12.5$. (From now on, we use indifferently T or β according to convenience.) The simplest choice was to run through this domain of the (H, T) plane along lines parallel either to the H axis or to the T axis, i.e., at fixed T or at fixed H, inasmuch as we could recover easily some of the thermodynamic quantities of interest by numerical computation of the derivatives with respect to the free variable.

We also expect that, given a hypothetical phase diagram for the infinite two-dimensional system, moving along a line of the (H, T) plane which is supposed to cross a transition line at a certain angle, the closer to a right angle that the intersection takes place, the clearer the announcement of the corresponding singularity will be reflected in the thermodynamic observables of the finite-width systems obtained by taking the derivative with respect to the moving coordinate.

Finally, we have explored the following lines:

(a) Constant temperature:

$$T/J = 0.32;\ 2;\ 5;\ 16/3;\ 8;\ 12.5$$

(H/J varying between -14 and $+2$).

(b) Constant applied field:

$$H/J = -2;\ -3\times 10^{-3};\ -2\times 10^{-3};\ -1\times 10^{-3};\ 0;\ 1\times 10^{-3};\ 2\times 10^{-3};\ 3\times 10^{-3}$$

(T/J varying between 0.25 and 12.5).

The reason for the set of small H/J values around zero was to allow for the determination of the magnetization and the susceptibility at zero field in addition to the thermal quantities and try to detect, if any, a transition at zero applied field when T varies.

(4) We have adopted the following criteria to ascertain a first-order phase transition in the infinite-width system: When crossing a first-order transition line in the phase diagram of the infinite system, one should observe a jump of m, U, and S, while χ and C should present a delta-function contribution in addition to their regular part. It is also known in this case that, in the corresponding finite-width systems, as n is increased, the amplitudes of χ and C at their largest value are expected to behave as $\exp(kn)$, contrasting with the n^{α} behavior observed in second-order transitions.

Therefore, we will adopt the following criterion: let $\chi_{n,J,T}(H)$ be the susceptibility as a function of H at fixed n, J, T; let $C_{n,J,H}(T)$ be the specific heat as a function of the temperature at fixed n, J, H. Then, if we are able to extract from the successive profiles of $\chi_{n,J,H}(H)$ [resp. $C_{n,J,H}(T)$] as n is increased a sequence of contributions that prefigure delta functions—i.e., peaks with increasing amplitudes and widths inversely proportional to their amplitudes—and if, moreover, these amplitudes follow an exponential behavior with respect to n, we conclude that in the limit where n goes to infinity the corresponding transition will be of first order.

5. Let us make a few general remarks about the results to be presented.

Due to the small number of values used for n, we do not pretend to present a thorough study of the problem. Although these values were sufficient in a limited number of cases to ascertain the existence of a first-order transition in the two-dimensional system, larger strips would have been necessary (if not sufficient) for a reliable conclusion in many cases, in particular if the onset of second-order transitions was suspected and required finite-size scaling analysis.

We also noted that the successive values of H for which $\chi_{n,J,T}(H)$ presents a maximum when n is increased do not form a monotonic sequence, due to the fact that because of the cyclic boundary conditions on the strips, the phase with three spins down and one spin up per elementary square, which represents a ground state of the infinite system when $-12 \leqslant H/J \leqslant -4/3$, cannot be achieved when n is odd. On the contrary, the sequences of T values for which $C_{n,J,H}(T)$ presents a maximum when n is increased are monotonic. These difficulties make it hard to determine precisely when a critical line (if critical) of the infinite system is being crossed over.

3.2. Presentation of the Results

For each of the two lines at constant temperature $T/J = 0.32$ and $T/J = 2$, a first-order transition is clearly evidenced, at a critical field H_c whose extrapolated value ($H_c \simeq -1.33J$ for $T/J = 0.32$; $H_c \simeq -1.26J$ for $T/J = 2$) is very close to the zero-temperature critical value $H_{c_1} = -\frac{4}{3}J$ predicted by the mean field theory. However, contrary to our expectations, no first-order transition shows up in the vicinity of $H_{c_2} = -12J$; even worse, at given temperature the susceptibility displays around this value a bump which remains practically constant in width and amplitude as a function of the size of the strip. The two cases $T/J = 0.32$ and $T/J = 2$ are illustrated by Figs. 7 and 8, respectively.

For the lines $T/J = 5$, 16/3, and 8, no positive conclusion about the nature of the transition corresponding to H_{c_1} can be given; for each of these temperatures, the maximum of susceptibility increases at increasing n, but no reliable law can be obtained. No sign of the transition corresponding to

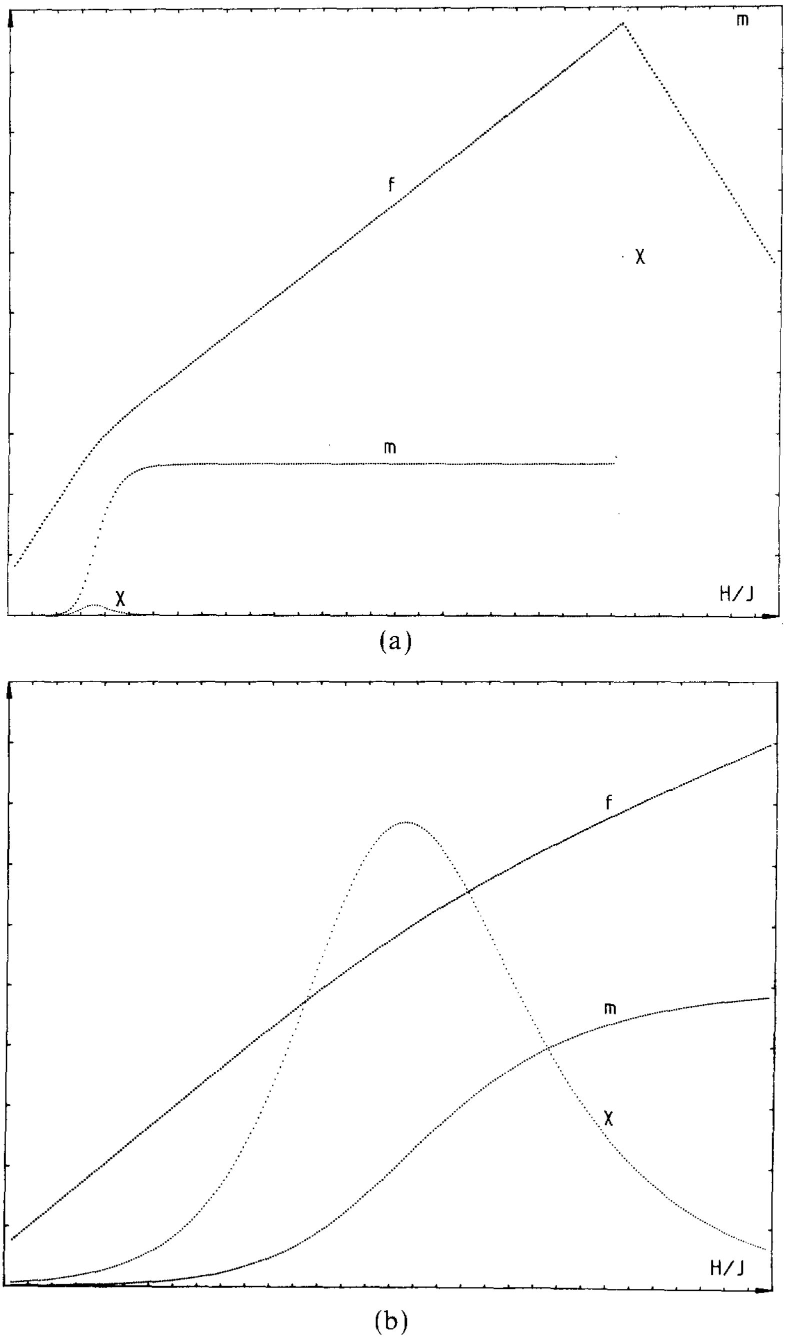
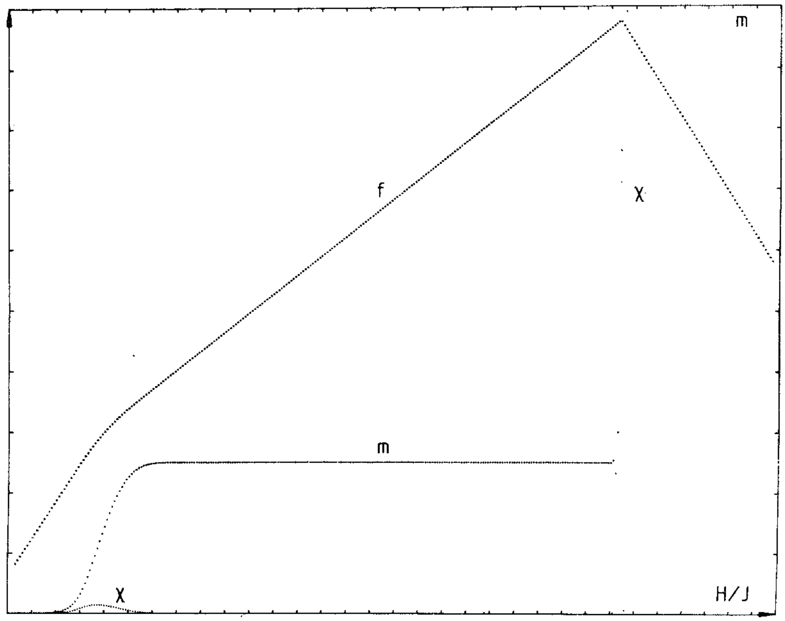
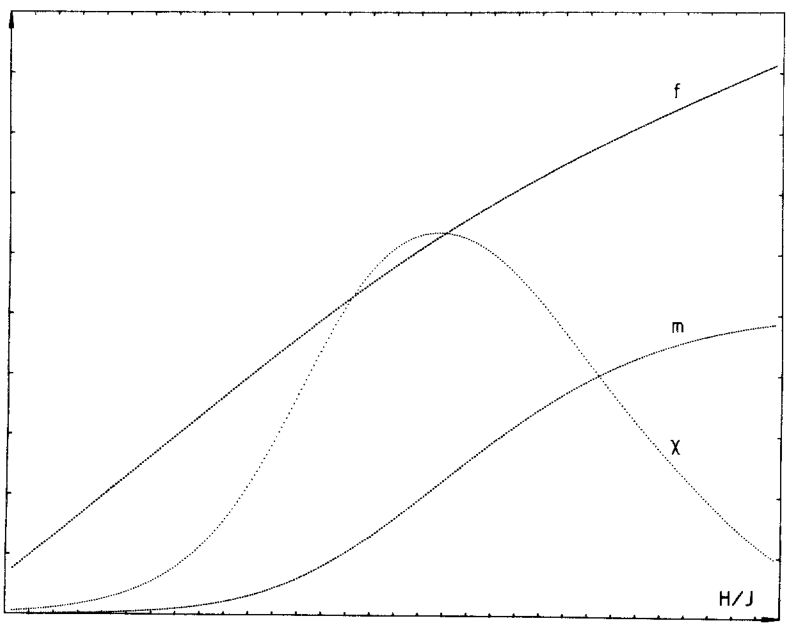


Fig. 7. Plots of free energy per spin, f, magnetization, m, susceptibility, χ, as functions of H/J at $T/J = 0.32$ for strips of different widths n. Respective scales of H/J, f, m, and χ are indicated in Table I. In (a), (c), and (e), the maximum value of χ is much larger than the corresponding upper scale 35, and χ appears practically as a delta-function profile. (a) $T/J = 0.32$, $n = 2$; (b) $T/J = 0.32$, $n = 2$, vicinity of $H/J = -12$; (c) $T/J = 0.32$, $n = 4$; (d) $T/J = 0.32$, $n = 4$, vicinity of $H/J = -12$; (e) $T/J = 0.32$, $n = 6$; (f) $T/J = 0.32$, $n = 6$, vicinity of $H/J = -12$.

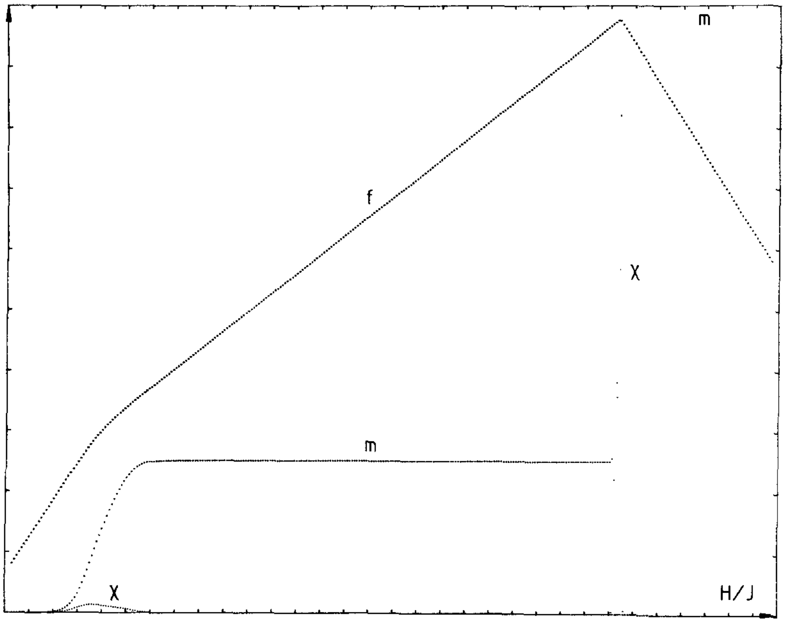


(c)

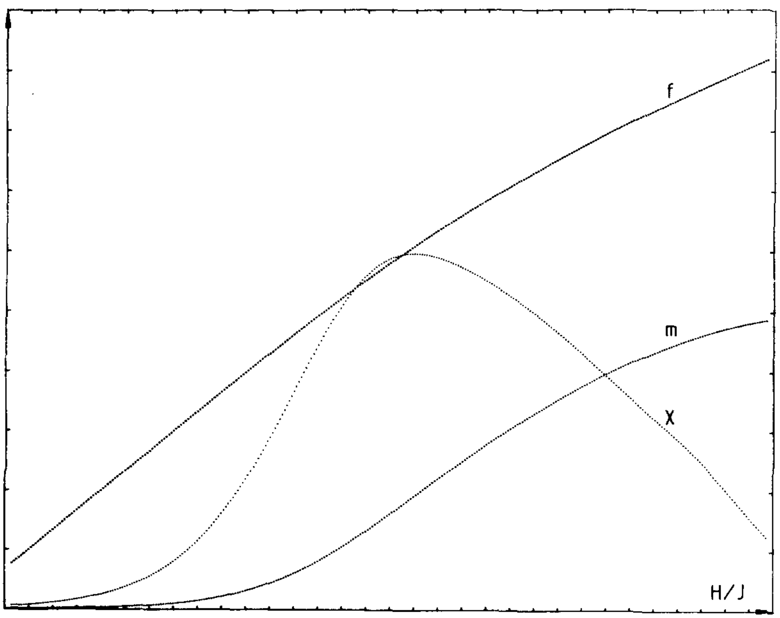


(d)

Fig. 7 (*continued*)

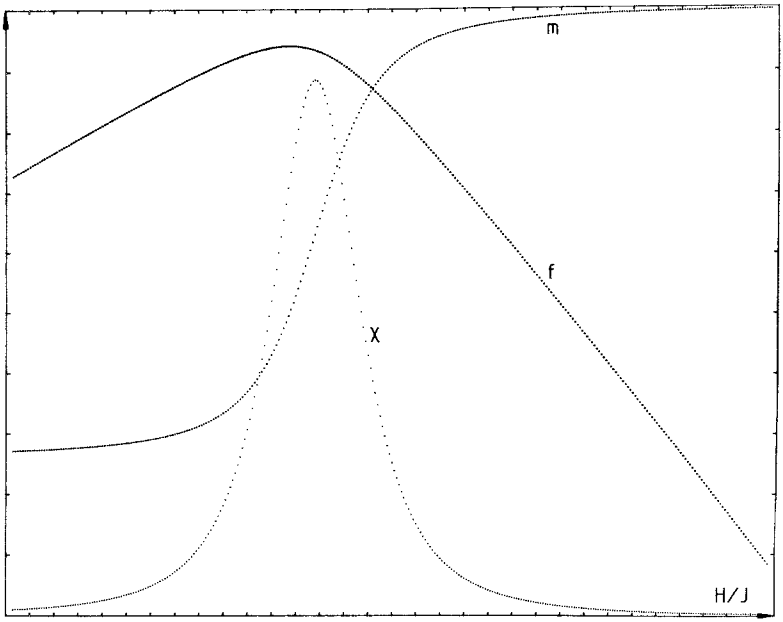


(e)

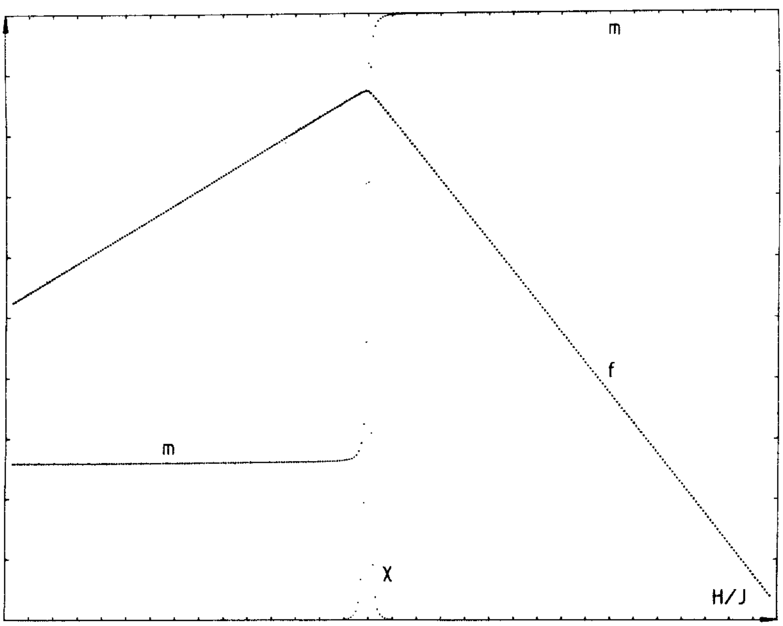


(f)

Fig. 7 (*continued*)

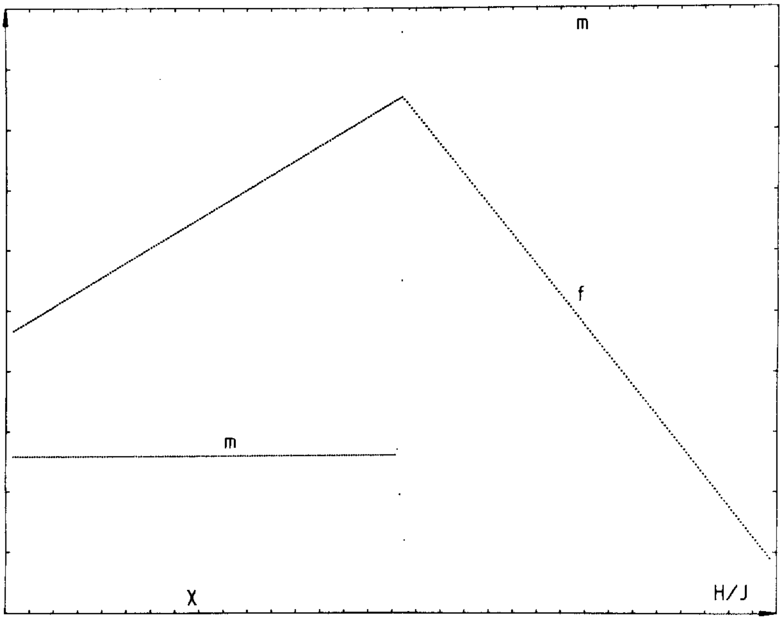


(a)



(b)

Fig. 8. Plots of free energy per spin, f, magnetization, m, and susceptibility, χ, as functions of H/J at $T/J=2.00$ for strips of different widths n. Respective scales of H/J, f, m, and χ are indicated in Table I. (a) $T/J=2.00$, $n=2$, $\chi_{\max}=13.28$ at $H/J=-1.064$; (b) $T/J=2.00$, $n=4$, $\chi_{\max}=275.3$ at $H/J=-1.200$; (c) $T/J=2.00$, $n=6$, $\chi_{\max}=5710$ at $H/J=-1.242$ (in this part, χ appears practically as a delta-function profile).



(c)

Fig. 8 (*continued*)

Table I

	H		f		m		χ	
Figure	min	max	min	max	min	max	min	max
7a	−14	2	−10.5	−2.5	−1	1	0	35
7b	−13	−11.4	−9.1	−7.6	−1	0	0	1
7c	−14	2	−10.5	−2.5	−1	1	0	35
7d	−13	−11.4	−9.1	−7.6	−1	0	0	1
7e	−14	2	−10.5	−2.5	−1	1	0	35
7f	−13	−11.4	−9.1	−7.6	−1	0	0	1
8a	−1.32	−0.68	−3.35	−2.95	−1	1	0	15
8b	−1.50	−0.86	−3.15	−2.75	−1	1	0	300
8c	−1.57	−0.93	−3.10	−2.70	−1	1	0	5750

H_{c_2} can be traced. For $T/J = 12$ a broad susceptibility bump of constant amplitude and width when n varies, centered at a positive value of the applied field, is observed.

Information from lines at constant field does not lead to definite conclusions. For the line at $H/J = -2$, the maximum of the specific heat increases with increasing n, but no reliable law of the value of this maximum versus n can be obtained (the extrapolated location of this maximum on the $H/J = -2$ axis is roughly $T/J \simeq 2.6$). For $H/J = 0$, both susceptibility and specific heat display the same type of behavior as in the previous case, with an extremum extrapolated at $T/J \simeq 5.5$ on the T axis.

With the elements we use, all we can state at this stage is that the phase diagram of the infinite, two-dimensional model contains a transition line which, in the (H, T) plane, begins at $H = -\frac{4}{3}J$, $T = 0$ with a very large (very likely infinite, as required by the Clausius–Clapeyron equation) positive slope and is definitely first order in the strip $0 \leqslant T/J \leqslant 2$. No convincing evidence for the existence of a second branch starting at $H = -12J$, $T = 0$ and encompassing what would be the NTI phase is available. Perhaps such a branch does not exist and the phase diagram would, like the pressure–temperature phase diagram of a fluid, exhibit only one first-order transition line, the NTI phase being inexistent. However, a preliminary investigation via Monte Carlo simulation seems to indicate that the NTI phase does indeed exist at low but not zero temperature,[11] so that if the NTI phase were to exist, at least part of the transition line ending at H_{c_2} would be second order. Incidentally, it may well be that the choice of order parameters used in Section 2 to describe the symmetry-breaking properties of the NTI phase could be improved, together with our understanding of the (possible) NTI–TI transition.

From our results, it is impossible to decide whether a transition takes place when the temperature varies at zero applied field (of course an exact solution of this case would be most welcome), so that we do not know if the first-order line starting at $H = H_{c_1}$, $T = 0$ does or does not cross the temperature axis.

4. CONCLUSION

We have studied the field–temperature phase diagram of a two-dimensional, three-spin interaction Ising model with a singlet ground state at zero field. This work has been done using two different methods: a mean field approximation and transfer matrice technique. Within the mean field framework we found two phases, one (TI) has the translational invariance of the underlying square lattice, and the other (NTI), enclosed in a finite domain, breaks this translational invariance. The "ordered" NTI phase presents some kind of residual disorder, but its number of ground states behaves as $N^{1/2}$. The NTI–TI phase transition is always first order. We also found inside the stability domain of the TI phase a first-order, liquid–gas-type phase transition characterized by a discontinuity of the magnetization. The corresponding line ends at a critical point and meets the NTI–TI transition line at a triple point.

These properties remain valid for a three-dimensional system, with the only difference that the NTI phase in this case is strictly periodic.

All the characteristic features of the phase diagram present striking similarities with those of a pure compound.

The numerical study by the transfer matrix method of two-dimensional finite-width systems confirms the existence of the first-order transition line for $-\frac{4}{3}J \leqslant H < 0$. For $H \leqslant -\frac{4}{3}J$, due to the insufficient maximum width of the strips, our results suggest two possibilities: either the NTI–TI phase transition is second order, or the NTI phase does not exist. This last possibility, however, seems to contradict a preliminary investigation by Monte Carlo simulations.

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