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CVM Modeling of the Square Ising Lattice with One Next-Nearest-Neighbor Interaction

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As an analysis of the development of first-order behavior in two-dimensional Ising lattices, the square lattice with antiferromagnetic nearest-neighbor interactions and a ferromagnetic next-nearest-neighbor interaction in the (11) direction has been modeled. The phase diagram was calculated for a range of interaction parameters and imposed fields; the calculations were performed using the cluster variation method (CVM). Analysis of the calculations suggests that no first-order behavior is developed in this system, so that higher dimensionality or connectivities are required before such behavior is developed.

KEY WORDS: Ising models; cluster variation method.

1. DESCRIPTION OF PROBLEM

The development of first-order behavior in two-dimensional systems is of fundamental interest in the study of lattice models and phase transitions. The ordering transition on the square lattice with only nearest-neighbor interactions is known to be second order under all conditions, whereas the square lattice with next-nearest-neighbor interactions in two directions develops a first-order transition for specific choices of nearest-neighbor and next-nearest-neighbor interaction parameters.[1] The present study considers the intermediate case of a square lattice with next-nearest-neighbor interactions in one direction only.

Recent work relating to this model includes that of Verhagen[2] and Wu,[3] each of which obtained solutions of the anisotropic triangular Ising lattice along particular trajectories in its parameter space; Wu's work is of

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particular interest inasmuch as the effect of a three-site interaction on the phase relations is considered. Expanding upon the solution of Verhagen, Rujan[4] analyzed the fully isotropic antiferromagnetic triangular lattice with nearest-neighbor interactions.

2. HAMILTONIAN

The Hamiltonian is

$$\mathscr{H} = -e_1 \sum_{i,j} \sigma_{i,j}(\sigma_{i+1,j} + \sigma_{i,j+1}) - e_2 \sum_{i,j} \sigma_{i,j}\sigma_{i+1,j+1} + H\mu \sum_{i,j} \sigma_{i,j}$$

where $\sigma_{i,j}$ represents a spin on the i, j lattice site, which can have value $+1$ or -1. The first sum is over nearest neighbors, whereas the second sum is over next-nearest neighbors in the single direction considered (Fig. 1), and the last term is a field term, which represents interaction between the spins and an imposed field; H is the field strength and μ is the coupling coefficient.

The behavior of the model in zero field ($H=0$) is well known; equilibrium long-range order (q) is given by the expression[5]

$$q^8 = 1 - \frac{(1-x_1^2)^4(1-x_2^2)^2}{16(1+x_1^2x_2)(x_1+x_2x_1)^2(x_2+x_1^2)}$$

where

$$x_i = \tanh(2e_i/kT)$$

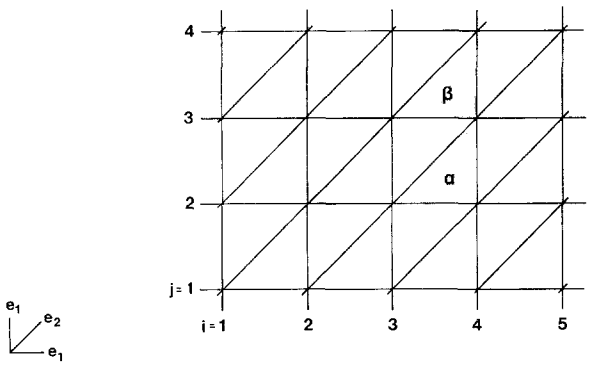

Fig. 1. Lattice numbering. e_1 and e_2 are nearest-neighbor and next-nearest-neighbor interactions, respectively. i and j are the two indices defining a site. Shaded triangles α and β represent the two basic clusters.

The present study is limited to cases subject to the constraint that the nearest-neighbor interactions (e_1) are equal in value and negative (antiferromagnetic), whereas e_2 is positive (or ferromagnetic). In this case, the ordered state ($T=0$) is rows [in the (11) direction] of parallel spins, the rows alternating in orientation; there is no bond frustration if $H=0$. This particular choice of interactions was chosen to relate most closely to the study of Nienhuis and Nauenberg[1]; other cases could be studied with little difficulty.

3. METHOD EMPLOYED

The phase diagram of this model was calculated using the cluster variation method (CVM) of Kikuchi[6] with two three-site triangles as basic clusters, illustrated as the shaded triangles α and β in Fig. 1. The CVM truncates the expression for the configurational entropy by considering only correlations among sites within a basic cluster, and so tends to overestimate transition temperatures because long-range correlations are ignored. The effect of chosing an alternative basic cluster will be discussed below.

The configurational entropy for the ordered phase is given by

$$S = Nk \ln(\Omega)$$

where Ω is the degeneracy factor, that is, the number of ways of constructing the system. The mechanics of constructing the degeneracy factor for a given lattice topology and basic cluster has been discussed by many authors.[6-8]

If one of the smallest triangles in Fig. 1 is chosen to be the basic cluster, and if we denote by P_i, H_{ij}, Y_{ij}, and T_{ijk} ($i, j, k = \pm 1$) the proportion of points, next-nearest-neighbor bonds, nearest-neighbor bonds, and triangles (respectively) with a given configuration, the degeneracy factor is found to be

$$\Omega = [H][Y]^2/[T]^2[P]$$

where

$$[T] = \prod_{i,j,k=\pm 1} (T_{ijk} N!)$$

and $[H]$, $[Y]$, and $[P]$ are defined analogously.

In the present case, the ordering scheme requires an expansion of the degeneracy factor; in the ordered phase, not all points, next-nearest-neighbor bonds, and points are equivalent. In particular (referring to

Fig. 1), points for which $i+j$ is odd are equivalent in the ordered phase, but not equivalent to those for which $i+j$ is even. The former set will be referred to as sublattice α and the latter as β, with configuration probabilities $P_{\alpha,i}$ and $P_{\beta,i}$, respectively. Next-nearest-neighbor bonds that link two α or β points are given configuration probabilities $H_{\alpha,ij}$ and $H_{\beta,ij}$, respectively, whereas triangles containing $H_{\alpha,ij}$ and $H_{\beta,ij}$ bonds are given configuration probabilities $T_{\alpha,ijk}$ and $T_{\beta,ijk}$, respectively. The expanded degeneracy factor is

$$\Omega = \frac{([H_\alpha][H_\beta])^{1/2}([Y_\alpha][Y_\beta])}{[T_\alpha][T_\beta]([P_\alpha][P_\beta])^{1/2}}$$

Note that the nearest-neighbor bonds (Y) are shared by both α and β triangles. Expansion of this term in the above expression is for computational and notational convenience; corresponding terms were constrained during the calculations.

The thermodynamic parameter minimized in the CVM is the grand potential:

$$\text{G.P.} = E - TS + H\mu \sum_{i,j} \sigma_{i,j}$$

The parameters of interest are the long-range order parameter q, which measures the perfection of the ordered phase and is defined as

$$q = \frac{P_{\alpha,1} - P_{\beta,1}}{P_{\alpha,1} + P_{\beta,1}}$$

and the short-range order parameters, which measure correlations between nearest neighbors (r_1) and between next-nearest neighbors (r_2), defined as

$$r_1 = Y_{1,1} + Y_{-1,-1} - Y_{-1,1} - Y_{1,-1}$$
$$r_2 = H_{1,1} + H_{-1,-1} - H_{-1,1} - H_{1,-1}$$

Note that r_1 and r_2 are defined separately for sublattices α and β, with appropriate choices of Y and H. Finally, the magnetization M is defined as

$$(P_{\alpha,1} + P_{\beta,1} - P_{\alpha,-1} - P_{\beta,-1})/2$$

4. RESULTS

Four different energy ratios were considered, $\log(-e_1/e_2) = -1$, 0, 1, and 1.5. For each energy ratio, isothermal sections were calculated at $T/T_c = 0.2$, 0.4, 0.6, and 0.8, as well as a polythermal section at $H = 0$.

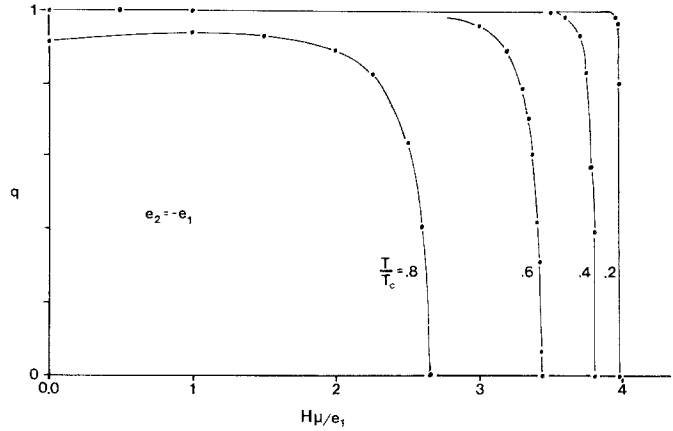

Fig. 2. Relation between long-range order q and imposed field H as a function of temperature T for the case $c_2 = -e_1$; T_c is the critical temperature of $H = 0$.

Figure 2 shows the relation between H and q for the case $e_2 = -e_1$; the other cases are qualitatively the same. The loss of long-range order becomes more abrupt at lower temperature; this may be extrapolated to a hypothetical first-order transition at absolute zero. For temperatures near T_c, q appears to increase slightly as H varies from zero to small values; this may be an artifact of the CVM and is in any case a small effect.

Figure 3 plots the relation between M and q for the same case. This

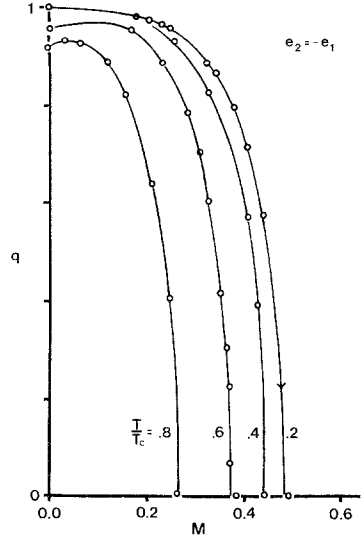

Fig. 3. Relation between long-range order q and magnetization M as a function of temperature for the case $e_2 = -e_1$; T_c is the critical temperature for $H = 0$.

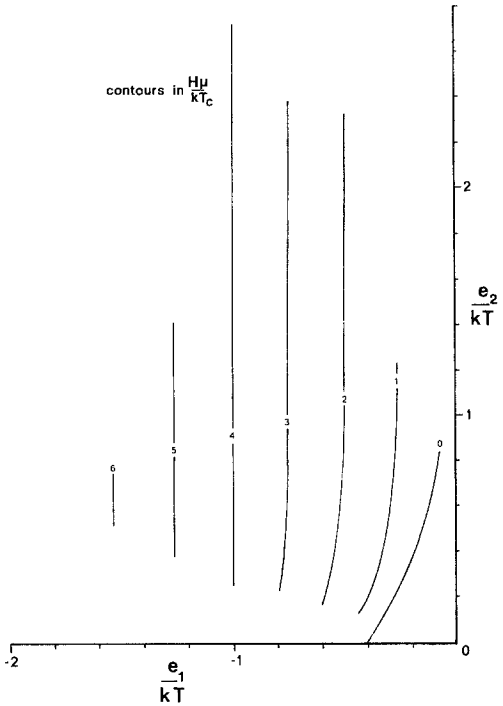

Fig. 4. Critical surface as a function of e_1/kT, e_2/kT, and $H\mu/kT_c$.

relation parallels that between H and q; q decreases continuously to zero as the M increases, and for T near T_c, q increases slightly as M diverges slightly from 0.0. Note that the limiting values of M in the ordered phase is 0.5; this is found in all cases.

Plotting the critical surface as a function of the two energy parameters (Fig. 4) and contouring in $H\mu/kT_c$, we note that as $-e_1/e_2$ decreases, the $H=0$ contour recedes to infinity as the lattice more closely approximates an ensemble of one-dimensional Ising lattices, which lack a phase transition. This contour crosses the abscissa at the calculated critical temperature of the simple square lattice and is within a few percent of the exact value.

5. SHORT-RANGE ORDER

The short-range order, in contrast to the long-range order, is finite for temperatures well in excess of the critical temperature. Figure 5 illustrates the specific case of $-e_1/e_2 = e^{1.5}$ and $H=0$. The variation of long-range order q with temperature is included for comparsion. Both short-range

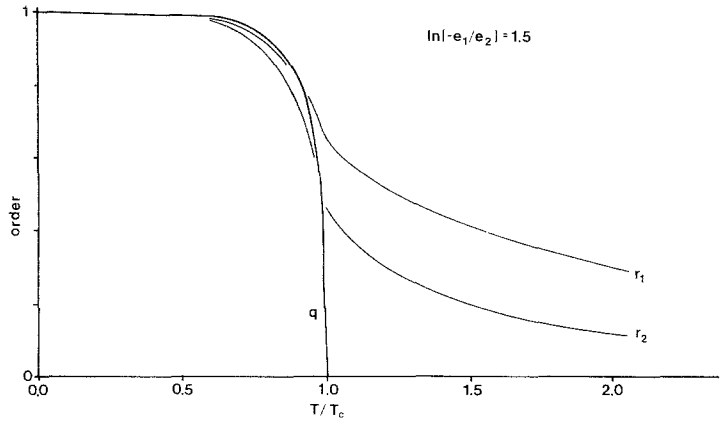

Fig. 5. Degree of order versus temperature T/T_c for the case $-e_1/e_2 = e^{1.5}$ and $H = 0$. The short-range order parameters r_1 and r_2 and long-range order parameter q are given. Note that as e_1 is negative (antiferromagnetic), the sign of r_1 is also negative—the absolute value has been plotted.

order parameters approach zero asymptotically as temperature increases, but at all temperatures the parameter r_1 is larger than r_2, because e_1 is the stronger interaction.

Each short-range order curve goes through an inflection at T_c, reflecting the qualitative change in the two-particle correlation function when long-range order is established.

6. FIRST-ORDER BEHAVIOR

The calculations were examined for evidence of a first-order transition; either a discrete change in slope of the grand potential versus imposed field relation at the transition point, or the coexistence of two phases of differing magnetization at the same value of imposed field. The examination revealed that neither criterion was met in any case, indicating that the transition is second order everywhere.

7. CONCLUSIONS

The phase diagram of the square Ising lattice with antiferromagnetic nearest-neighbor interactions and ferromagnetic next-nearest-neighbor interactions in one direction has been solved in the two-triangle CVM approximation. The phase diagram shows a second-order transition at all temperatures and ratios of interaction energies; there is no evidence of first-order behavior. This result, considered in the light of earlier work,[1]

indicates that first-order behavior is only developed at higher dimensionalities and/or lattice connectivities than this lattice. In particular, it appears that the addition of the second next-nearest-neighbor interaction is necessary for first-order behavior to be developed in two dimensions. The two-triangle approximation is minimal for this lattice; the accuracy of the phase diagram would be improved by a choice of a larger basic cluster, e.g., a nine-point quadruple square; however, the calculations performed in this study and analysis of the modeling procedure suggest that further modeling of this lattice would not significantly change the conclusions. It is worth noting that the study of Kurata *et al.*[9] suggests that the results obtained by using a two-triangle rhombus (i.e., an α and a β triangle joined along a nearest-neighbor bond) would be identical to the present results.

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