Phase boundary of the two-dimensional Ising model with ferromagnetic and antiferromagnetic interactions in a magnetic field

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The interface method is used to derive the order-disorder critical temperature of the two-dimensional Ising model on a rectangular lattice with ferromagnetic interactions in the x direction and antiferromagnetic interactions in the y direction. Employing this approximation in two different ways gives different critical temperatures T_c for nonzero uniform magnetic fields H. However, both of the phase boundaries $T_c(H)$ reduce to the exact results available at $H=0$ and $T=0$.

I. THE MODEL AND ITS PHASES

Two-dimensional Ising models in magnetic fields have been used extensively to study a variety of experimental systems.[1] Here I investigate this model on a rectangular lattice when near-neighbor interactions in the two perpendicular directions, J_x and J_y, have *different* signs.[2] Further-neighbor interactions are neglected. Despite its simplicity, this case has received little attention.[3]

The Hamiltonian $\mathcal{H}$ may be written as

$$\mathcal{H}=-J_x\sum_{i,j}\sigma_{i,j}\sigma_{i+1,j}+J_y\sum_{i,j}\sigma_{i,j}\sigma_{i,j+1}-H\sum_{i,j}\sigma_{i,j}\ , \quad (1)$$

where i is taken to be along the x axis, j along the y axis, and the Ising variables $\sigma_{i,j}$ take on the values ± 1. In the case of interest here, both J_x and J_y are positive, while H may be of either sign.

The ground-state analysis of Eq. (1) is straightforward. Ferromagnetic states are found for $|H|>2J_y$, corresponding to all $\sigma_{i,j}=1$ for $H>2J_y$ or all $\sigma_{i,j}=-1$ for $H<-2J_y$. For $|H|<2J_y$, two degenerate ground states are possible. The one chosen here has $\sigma_{i,j}=1$ for even j and -1 for odd j. This state may be described as ferromagnetic chains, aligned along the x axis, coupled antiferromagnetically (in the y direction.) Upon introducing the temperature T, a transition is present (for $|H|<2J_y$) between the low-T, "striped," ordered (2×1) phase and the high-T, (1×1) ferromagnetic phase. In this paper the phase boundary, $T_c(H)$, between the phases with these two symmetries will be investigated.

II. PREVIOUS RESULTS

For $H=0$, T_c solves the equation first derived by Onsager:[4]

$$\sinh[2J_x/(k_BT_c)]\sinh[2J_y/(k_BT_c)]=1\ .$$

Approximations are needed to perform the statistical mechanics to determine $T_c(H)$ for nonzero H.

Conventional mean-field theory,[5] when applied to this case, is both qualitatively and quantitatively wrong. It predicts a first-order transition for small[6] T. However, the actual boundary is expected[7] to be second-order (of the Ising universality class) for all T. At high T, mean-field theory[5] predicts a second-order transition, with T_c solving

$$H=2(J_x+J_y)m+\tfrac{1}{2}k_BT_c\ln\frac{1+m}{1-m}\ ,$$
$$m=\left[1-\frac{k_BT_c}{2(J_x+J_y)}\right]^{1/2}\ . \quad (2)$$

At $H=0$, $k_BT_c=2(J_x+J_y)$, which disagrees significantly with the exact result.[4] For example, for $J_x=J_y\equiv J$, Eq. (2) gives $k_BT_c(H=0)=4J$, which is nearly a factor of 2 larger than the exact result, $k_BT_c(H=0)=2J/\ln(1+\sqrt{2})$.

It is also possible to investigate the phase diagram using the linear-chain approximation.[7] In this method the statistical-mechanics analysis is taken as exact along the chains and in a mean-field sense between the chains. The analysis is appropriate at low T, and a second-order transition is found.

Finally, this diagram may also be studied using the free-fermion approximation. In this method the stringlike low-temperature excitations of the striped phase are treated as worldlines of fermions. Although the main emphasis of previous work[8] involves other boundaries found in a model with an additional term, results relevant to model (1) are also included in these studies.

III. APPLICATION OF THE INTERFACE METHOD

The interface method of Müller-Hartmann and Zittartz[9] has often been used to estimate second-order phase boundaries of two-dimensional models. The method, which predicts only second-order boundaries, is appropriate here because, when further-neighbor interactions are excluded, the boundaries are expected to be second order. The original application of this method to the square-lattice Ising antiferromagnet was conjectured to give exact results. Further analysis has shown that the method is not exact (for $H\neq 0$) in this case.[10] Yet Monte Carlo simulations often have sufficiently large error bars that they agree with this conjecture.[11]

In applying this method, the interface free energy between the two coexisting (low-T) phases is considered. An approximation to the interface free energy σ is calculated by including solid-on-solid fluctuations of the interface. For this restricted set of configurations, σ can be found exactly using transfer-matrix methods. Setting $\sigma=0$ gives the transition temperature in question. This method is intriguing because it gives exact results for the anisotropic near-neighbor Ising model at $H=0$, independent of the signs of J_x and J_y.

This method is applied to our model in two different ways. In both cases the stripes of both coexisting phases are aligned in the x direction. Previously[12] the interface method was applied to the striped phase which is present in the *isotropic* square-lattice Ising model with both nearest- and next-nearest-neighbor interactions. In that work, application to the interface between domains in which the stripes were oriented perpendicularly to each other resulted in a phase boundary which was discarded since it disagreed with the known ground state.

In the first case the interface is taken to be oriented parallel to the stripes with a unit normal in the y direction. The ground-state interface, with two adjacent $\sigma_i=1$ chains, has energy $E_0=2NJ_y-NH$, where N is the number of columns. If the ith column has column height n_i, then the excess interface energy (above E_0) associated with the configuration $\{n_i;\, i=1,\ldots,N\}$ of column heights is given by

$$\Delta E=2J_x\sum_i |n_i-n_{i+1}|+H\sum_i[1-(-1)^{n_i}]\,. \tag{3}$$

The largest eigenvalue of the associated transfer matrix is

$$\lambda=\frac{e^{-B}}{\sinh(2K_x)}[\cosh B\cosh K_x+(1+\sinh^2 B\cosh^2 K_x)^{1/2}]\,, \tag{4}$$

where $B=H/(k_BT)$ and $K_{x,y}=2J_{x,y}/(k_BT)$. Setting $\sigma=E_0/N-k_BT\ln\lambda$ equal to zero gives the following equation which T_c solves:

$$\cosh B=\sinh K_x\cosh K_y/\cosh K_x\,. \tag{5a}$$

Equation (5a) may be rewritten as

$$\sinh K_x\sinh K_y=(1+\sinh^2 B\cosh^2 K_x)^{1/2}\,. \tag{5b}$$

In the second case the interface is oriented perpendicular to the chains with a unit normal in the x direction. The ground-state energy is now $E_0=2NJ_x$, while the excess energy becomes

$$\Delta E=2J_y\sum_i |n_i-n_{i+1}|+2H\sum_i(-1)^i n_i\,. \tag{6}$$

The associated eigenvalue is

$$\lambda=\frac{\sinh K_y}{\cosh K_y-\cosh B}\,, \tag{7}$$

so T_c satisfies

$$\cosh B=\cosh K_y-\exp(-K_x)\sinh K_y\,, \tag{8a}$$

or, equivalently,

$$\sinh K_x\sinh K_y=\cosh B+\tfrac{1}{2}\frac{\sinh^2 B}{\cosh K_y-\cosh B}\,. \tag{8b}$$

The difference in phase boundaries (5) and (8) is not unexpected, since previous applications of this method also give results that depend on the interface orientation when at least one of the phases has a striped or more complicated structure.[12,13]

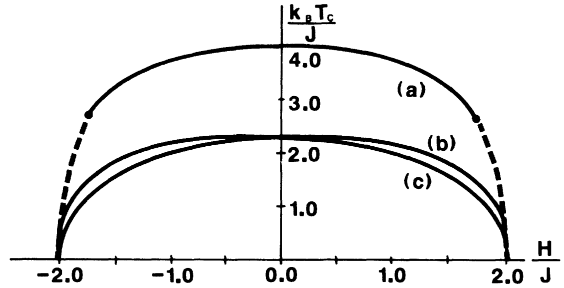

FIG. 1. Phase diagrams for the anisotropic Ising model of Eq. (1) with $J_x=J_y\equiv J$, where J_x is the ferromagnetic interaction in the x direction and J_y is the antiferromagnetic interaction in the y direction. The curve derived from mean-field theory (a) incorrectly gives first-order boundaries (dashed curves) at low temperatures and a T_c near $H=0$ which is too large by nearly a factor of 2. The boundaries b and c are found using two versions of the interface method and are solutions of Eqs. (5) and (8), respectively. These boundaries are exact at $H=0$ and expected to be fairly close to the exact boundaries.

In Fig. 1 the phase boundaries for $J_x=J_y\equiv J$ are plotted using both versions of the interface method [Eqs. (5) and (8)] as well as conventional mean-field theory.[5] All three curves agree with the exact ground-state analysis, while only the two curves based on the interface method agree with the exact result[4] at $H=0$. For small T, Eq. (5) becomes $H=2J_y-2k_BT\exp(-2K_x)$, while Eq. (8) becomes $H=2J_y-k_BT\exp(-K_x)$. It is interesting to note that, at low-T, the linear-chain approximation[7] gives the curve

$$H=2J_y+(J_yk_B^2T^2/4)^{1/3}\exp(-2K_x/3)\,,$$

which bulges in the opposite direction, while the free-fermion approximation[8] predicts $H=2J_y-k_BT\times\exp(-4K_x)$, which bulges in the same direction but disagrees with both low-T results. Near $H=0$, $T_c(H)\cong T_c(0)-\frac{1}{2}\kappa H^2$, where $\kappa=-k_B\partial^2T_c/\partial H^2|_{H=0}$. From Eq. (5),

$$\kappa=\tfrac{1}{2}\cosh^2 K_x(J_x\coth K_x+J_y\coth K_y)^{-1}\,,$$

while Eq. (8) gives

$$\kappa=[2(\operatorname{sech}K_y-1)(J_x\coth K_x+J_y\coth K_y)]^{-1}\,.$$

Mean-field theory gives $\kappa=1/[4(J_x+J_y)]$. For Fig. 1, $\kappa J=1/8$, $1/(2\sqrt{2})$, and $1/[4(\sqrt{2}-1)]$ for curves a, b, and c, respectively.

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