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Phase Diagram of the Antiferromagnetic Triangular Ising Model with Anisotropic Interactions*

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It is argued that there exist two antiferromagnetic phases in the triangular Ising model with anisotropic interactions. A method due to Müller-Hartmann and Zittartz (MZ) is used to derive a closed-form expression for the phase boundary. We also give a criterion under which the MZ method is expected to be applicable and accurate.

I. Introduction

It is well-known that the antiferromagnetic triangular Ising model with isotropic interactions exhibits no phase change [1]. There is no exact result on the antiferromagnetic triangular Ising model when there is a nonzero magnetic field, but the current belief is that the phase diagram of the isotropic model is as shown in Fig. 1 [2, 3]. The situation is less clear when the interactions are anisotropic. While it is known that the anisotropy does bring about a nonzero Néel point [4], the effect of an external magnetic field has not been adequately examined. We look into this problem in this paper. We shall see that a new feature, which emerges as a result of the anisotropy, is the existence of two antiferromagnetically ordered phases characterized by different ground state spin arrangements. In fact, we shall derive a closed-form expression for the boundary between these two phases. The derivation is based upon a method due to Müller-Hartmann and Zittartz (MZ) [5] for the square lattice, and we conjecture as in MZ that the phase boundary so obtained is exact. We also discuss briefly why the MZ method gives excellent result in some models while failing in others.

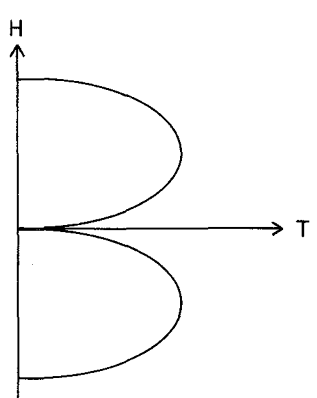

Fig. 1. Conjectured phase diagram for the isotropic antiferromagnetic Ising model on the triangular lattice. H is the external magnetic field

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II. Triangular Ising Model

Consider an Ising model on a triangular lattice with the Hamiltonian

$$\mathscr{H}=\sum_{\alpha=1}^{3} J_\alpha \sum^{(\alpha)} \sigma_i \sigma_j - H \sum \sigma_i. \tag{1}$$

Here H is the external magnetic field, and $\sum^{(\alpha)}$ denotes summation over nearest-neighboring pairs in the direction $\alpha(=1,2,3)$. We have also adopted the convention that $J_\alpha>0$ denotes antiferromagnetic interactions. For $H=0$ the triangular Ising model exhibits a unique critical point [4]. To discuss the situation it is most convenient to consider the triangular Ising model as a free-fermion model [6] on the square lattice. The critical point is then conveniently given in terms of the vertex weights [6]

$$\begin{aligned}
\omega_1&=\exp[-(J_1+J_2+J_3)/kT],\\
\omega_2&=\exp[(J_1+J_2-J_3)/kT],\\
\omega_3&=\exp[(J_1-J_2+J_3)/kT],\\
\omega_4&=\exp[(-J_1+J_2+J_3)/kT]
\end{aligned} \tag{2}$$

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as

$$\omega_1+\omega_2+\omega_3+\omega_4=2\max\{\omega_1,\omega_2,\omega_3,\omega_4\}. \qquad (3)$$

The expression (3) is very concise, and is valid for all values of J_α. There is no phase transition ($T_c=0$) if the two largest ω's are equal. This will happen if either all three J's are equal and positive, or one is positive while the remaining two are equal and smaller in magnitude. We shall consider the case in which, in the absence of an external magnetic field, the ground state of (1) is nonferromagnetic. Without loss of generality, we may take the ground state to be one in which pairs of spins interacting with J_3 are parallel, while those interacting with J_1 or J_2 are antiparallel. By comparing the energies it is seen that this is the case if

$$J_1+J_2\geqq 0, \quad J_1\geqq J_3, \quad J_2\geqq J_3. \qquad (4)$$

Here the larger of J_1 and J_2, say J_1, must be positive (antiferromagnetic), while J_2 and J_3 can be either positive or negative. We shall henceforth consider the Ising model under the restriction of (4). The critical condition (3) now reads $\omega_2=\omega_1+\omega_3+\omega_4$ or, explicitly.

$$e^{2K_3}=\sinh(K_1+K_2)/\cosh(K_1-K_2), \qquad (5)$$

where $K_i=J_i/kT$.

Orient the lattice as shown in Fig. 2. We next examine the ground state configuration for $H\neq 0$. It is clear that for large $|H|$ the ground state is ferromagnetic. This situation is shown in Fig. 3a. For smaller values of $|H|$, it turns out that either the configuration (b) or the configuration (c) of Fig. 3 may have the lowest energy. A little calculation shows that, for $J_3>0$,

(A) $E_a<E_b, E_c, \quad |H|>2(J_1+J_2+J_3)$

(B) $E_b<E_a, E_c, \quad |H|<2(J_1+J_2)-4J_3$

(C) $E_c<E_a, E_b,$

$$2(J_1+J_2)-4J_3<|H|<2(J_1+J_2+J_3) \qquad (6)$$

and, for $J_3<0$,

(A) $E_a<E_b, E_c, \quad |H|>2(J_1+J_2)$

(B) $E_b<E_a, E_c, \quad |H|<2(J_1+J_2)$. (7)

Here E_a is the energy of the configuration shown in Fig. 3a, E_b that of Fig. 3b, etc. Thus, as $|H|$ increases, the ground state undergoes two transitions for $J_3>0$ and one transition for $J_3<0$. We also point out that the spin state of Fig. 3b is doubly degenerate, while that of Fig. 3c is triply degenerate.

Now we ask what happens if the temperature is raised from absolute zero. Unfortunately, not much is known in this region. However, on the basis of what has been established for the square lattice [2, 3, 5] and on

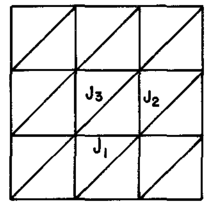


Fig. 2. Orientation of the triangular lattice

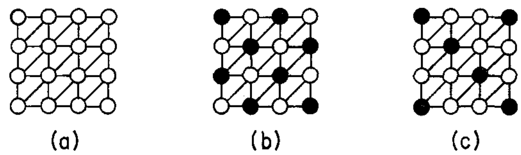


Fig. 3 a – c. Possible ground state spin arrangements. White (black) circles denote $+(-)$ spins for $H>0$, and $-(+)$ spins for $H<0$. **a** Ferromagnetic, nondegenerate. **b** Antiferromagnetic, doubly degenerate. **c** Antiferromagnetic, triply degenerate. The black circles are one of the three sublattices

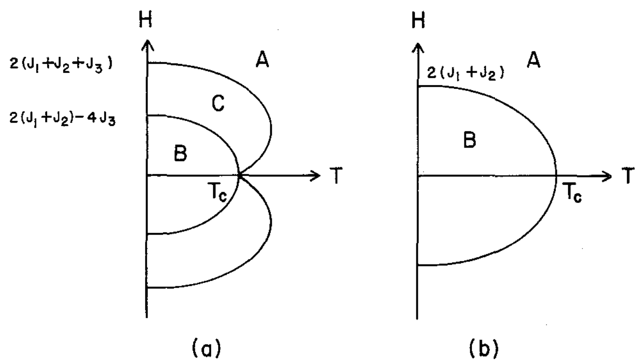


Fig. 4a and b. Phase diagram (schematic) for the triangular Ising model specified by (4). **a** $J_3>0$. **b** $J_3<0$

intuitive grounds, we expect the phase boundary to extend to nonzero temperatures. Furthermore, we know that there exists a unique critical temperature T_c for $H=0$. We then expect the phase diagram to behave as shown in Fig. 4, namely, there exist two antiferromagnetically ordered phases for $J_3>0$ and a unique antiferromagnetic phase for $J_3<0$. Here the regions A, B, and C in Fig. 4 correspond to those in (6) and (7).

We shall in the following obtain a closed-form expression for the boundary of region B. For continuity in reading, we first give this expression and examine its implications. The derivation will be given subsequently. The boundary of region B in both Fig. 4a and Fig. 4b is found to be

$$e^{4K_3}=[\cosh 2(K_1+K_2)-\cosh L]/[\cosh 2(K_1-K_2)+\cosh L], \qquad (8)$$

where $L=H/kT$. We have been unable, however, to obtain an expression for the boundary between regions A and C in Fig. 4a.

It is readily seen that (8) yields all known results. For $H=0$ (8) reduces to the exact critical condition (5). For $J_3=0$, the region C in Fig. 3a is expected to vanish, as is already evident in (6). This is the square lattice and there is now only one phase boundary which becomes

$$\sinh 2K_1 \sinh 2K_2 = \cosh L, \tag{9}$$

in agreement with the result of MZ [5]. Finally, when the interactions are isotropic, $J_\alpha = J > 0$, one verifies that the condition (8) is satisfied only by $H=T=0$ so that region B in Fig. 4a disappears by shrinking into a single point at the origin. Thus, the phase diagram reduces to that of Fig. 1. Another situation of interest is the case of $J_1 > J_2 = J_3 > 0$ for which $T_c = 0$ with region B shrinking into the line segment $|H| < 2J_1 - 2J_2$ along the $T=0$ axis. We also obtain the following expansions:

$$T_c(H) = T_c(0) - O(H^2), \qquad H \to 0, \tag{10}$$

$$H = H_c - O(T_c e^{-c/T_c}), \qquad T_c \to 0, \qquad J_3 \neq 0, \tag{11}$$

where c is a constant, and

$$\begin{aligned} H_c &= 2(J_1+J_2) - 4J_3, \qquad J_3 > 0 \\ &= 2(J_1+J_2), \qquad J_3 < 0. \end{aligned} \tag{12}$$

We point out that the critical field has an exponential decay for small T_c; this is different from the linear dependence found for $J_3=0$ [5].

We now sketch the derivation of (8), which differs slightly from that of MZ. Consider an $N \times \infty$ lattice as arranged in Fig. 2 [7]. Following MZ [5], we specify an arbitrary interfacial configuration by the height n_i ($=0, \pm 1, \pm 2, \ldots, \pm \infty$) at which the interface separates the two degenerate ground states in column i ($=1, 2, \ldots, N$). The boundary condition of $n_1 \equiv n_{N+1} = 0$ is used in MZ. To make the derivation more transparent, we shall relax the boundary condition by letting *all* n_i to take on all possible values. As we shall see, any difference this introduces will disappear in the thermodynamic limit. Let $T(L)$ be the transfer matrix which transfers from column to column. Then, following the development of MZ, we arrive at the following expression for the surface tension along a transverse boundary:

$$\sigma = -kT \ln \sqrt{\lambda_1}, \tag{13}$$

where λ_1 is the largest eigenvalue of the matrix

$$W = T(L)\, T(-L). \tag{14}$$

The critical condition is now obtained by setting $\sigma = 0$ or simply

$$\lambda_1 = 1. \tag{15}$$

The matrix elements of $T(L)$ are obtained by explicitly writing down the interaction energy between two neighboring columns of spins with interface heights m and n. Taking the doubly degenerate spin states of Fig. 3b as the two ground states separated by the interface, we obtain similarly to MZ the following expression for the matrix elements:

$$\begin{aligned} T_{mn}(L) \equiv [T(L)]_{mn} = \exp\{&-2K_2 - 2(K_1-K_3)|m-n| \\ &+ \tfrac{1}{2} L[(-1)^m - (-1)^n] + \Delta_{mn}\}. \end{aligned} \tag{16}$$

with

$$\begin{aligned} \Delta_{mn} &= -2K_3, \qquad m < n \\ &= 2K_3, \qquad m \geqq n. \end{aligned}$$

Now $W_{mn} = W_{m+2,n+2} > 0$ for all m, n. It then follows from the Perron-Fröbenius theorem that λ_1 is the larger of the two eigenvalues of the 2×2 matrix Λ [8] whose elements are

$$\Lambda_{\alpha\beta} = \sum_{k=-\infty}^{\infty} W_{\alpha, 2k+\beta}, \qquad \alpha, \beta = 1, 2. \tag{17}$$

Introducing (14), we find

$$\Lambda = t(L)\, t(-L), \tag{18}$$

where

$$t_{\alpha\beta}(L) = \sum_{k=-\infty}^{\infty} T_{\alpha, 2k+\beta}(L). \tag{19}$$

Using (16), we obtain from (19)

$$t(L) = \begin{pmatrix} A_1 & A_3 e^{L} \\ A_3 e^{-L} & A_1 \end{pmatrix}, \tag{20}$$

where

$$A_i = e^{-2K_2} \cosh 2K_i / \sinh 2(K_1 - K_3). \tag{21}$$

It follows that

$$\Lambda = \begin{pmatrix} A_3 e^{L} & A_1 \\ A_1 & A_3 e^{-L} \end{pmatrix}^2. \tag{22}$$

The critical condition (15) now becomes

$$A_1^2 - A_3^2 + 2A_3 \cosh L = 1 \tag{23}$$

which leads to (8) upon using (21).

III. Discussions

We have examined the phase diagram for the antiferromagnetic triangular Ising model with anisotropic interactions, and obtained an expression for its phase boundary. Since the method of MZ of computing the interfacial tension is by itself an approximation, it is remarkable that the resulting expression does agree with all the known results. As in MZ, we suppose that the errors involved in the procedure somehow cancel, and conjecture that the phase boundary (8) is in fact exact. Now the derivation of (8) uses explicitly the fact of the coexistence of two doubly degenerate ground states. It follows that the boundary so obtained is that of region B. It is also for this reason that the MZ method is not suitable for obtaining the phase boundary between regions A and C, for which a triply degenerate spin state is involved. Clearly, some generalization of the MZ method is needed in order to make further progress in this direction.

Our procedure also leads to an explicit expression for the interfacial tension σ for all H. For $H=0$ this expression reduces to the zerofield interfacial tension along an interface perpendicular to J_2 as obtained by Southern [9], who also used the MZ method to compute σ. For $H \neq 0$, however, our expression is not symmetric in J_1 and J_3, and presumably is a poor approximation to the interfacial tension along the same interface. It also does not lead to the exact result of Fisher and Ferdinand [10] for the ($H=0$) interfacial tension along the J_1 axis except in some special cases. Apparantly, as already noted by Burkhardt [11], the MZ method is more useful in determining the critical point, which presumably depends less critically on the choice of the interfacial boundary. However, despite of its apparent success in the present problem, the MZ method does not lead to the correct critical point in other problems such as the Baxter 8-vertex model and the Ashkin-Teller model. An immediate question is to ask whether there exists any criterion for its application?

A partial answer to this question is the following. To help to visualize the situation, let us consider more generally an 8-vertex model as defined in Fig. 5. By taking special values for the vertex weights ω_i, staggered if necessary, this model generates, among others, the n.n. and n.n.n. Ising model [12], the Baxter 8-vertex model [13], the Ashkin-Teller model [14], and the Potts model [15]. It is therefore sufficiently general for the purpose of our discussion. Now, each bond configuration of the 8-vertex model can be mapped into two degenerate spin states by placing spins on the dual lattice and considering the bonds as separating antiparallel spins [16]. Assume ω_1 to be the largest vertex weight. Then the ground state of the spins is ferromagnetic and the bonds can be thought of as the interfacial boundary. It is now possible to apply straightforwardly the MZ method to this problem. In the MZ procedure only those interfaces which do not contain border crossings are considered. As a result, the vertex weight ω_2 of the crossover configuration in Fig. 5

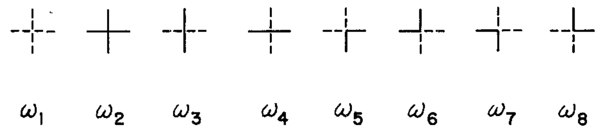
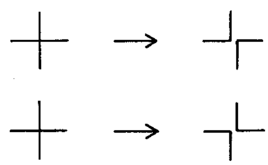


Fig. 5. General 8-vertex model with arbitrary vertex weights



$\omega_1 \omega_2 = \omega_5 \omega_6$

$\omega_1 \omega_2 = \omega_7 \omega_8$

Fig. 6. Decomposition of a crossover vertex configuration into noncrossing borders

never enters the picture; the phase boundary so derived is independent of ω_2. Certainly, this cannot be correct for all ω_2. It is for this reason that the MZ procedure will in general yield poor results for the 8-vertex model. However, if we have either

$$\omega_1 \omega_2 = \omega_5 \omega_6 \quad \text{or} \quad \omega_1 \omega_2 = \omega_7 \omega_8, \tag{24}$$

then we may decompose the crossover configuration into two noncrossing borders as shown in Fig. 6, while at the same time retaining the correct relative weights for the noncrossing borders. Thus, we are in effect considering only noncrossing interfaces. Consequently, the condition (24) can be taken to be a criterion under which the MZ procedure is expected to be most accurate. This condition also serves to single out *one* value of ω_2 for which the MZ method is reasonable and legitimate.

Now, for the triangular (and the square) Ising model, the vertex weights of the corresponding 8-vertex model [6] indeed satisfy (24). Therefore, it is not accidental that good results are obtained in these cases. As a matter of fact, the vertex-model formulation of the Ising model is more revealing. Considered as a free-fermion model [6], the derivation of the critical condition follows a more elegant course and leads to the expression

$$2 \cosh L = (\omega_1^2 + \omega_2^2 - \omega_3^2 - \omega_4^2)/(\omega_1 \omega_2 + \omega_3 \omega_4). \tag{25}$$

The expression (25), which reduces to (8) upon using (2), reflects the full symmetry of the problem. For other problems such as the Baxter 8-vertex, Ashkin-Teller, and the Potts models, the condition (24) does not hold. Consequently, the MZ method is a poor approximation and is not expected to lead to reliable results.

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8. Let $\Lambda\begin{pmatrix}a\\b\end{pmatrix}=\lambda_1\begin{pmatrix}a\\b\end{pmatrix}$, then $W\psi=\lambda_1\psi$ where $\tilde{\psi}=(a, b, a, b, \dots)$. The Perron-Fröbenius theorem now implies that λ_1 is the larger eigenvalue of Λ if, and only if, λ_1 is the largest eigenvalue of W
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