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Triangular antiferromagnetic Ising model*

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We solve the Ising problem on a triangular lattice with anisotropic interactions. Special consideration is given to the antiferromagnetic case. It is found that no phase transition exists if $J_1 = J_2 = J_3 < 0$. Allowing a slightly different value of one of the coupling constants J_3, we find $kT_c \simeq 2(|J_1| - |J_3|)/\ln 2$ if $|J_3| - |J_1| \to 0^-$, while no phase transition exists if $|J_3| > |J_1|$. Physical arguments to explain this behavior are also presented.

I. INTRODUCTION

The importance of the Ising model as one of the very few exactly soluble many-body problems with a phase transition is well known and need not be reviewed here. After the famous Onsager solution,[1] much work has been done to simplify the derivation and extend to results to other planar lattices.[2-6] The critical temperature on a square lattice, in particular, was found by Kramers and Wannier[7] even before Onsager's exact solution. The model presents in all cases a logarithmic singularity in the specific heat at a critical temperature which varies from lattice to lattice.

For lattices like the square or hexagonal, on which every closed loop has an even number of bonds, the thermodynamic functions in zero field turn out to be even functions of J; thus, no special consideration is required for the antiferromagnetic case. The reason is clear: The change $J \to -J$ is obtained by changing $\sigma \to -\sigma$ on one of the two sublattices into which the original lattice can be split. The purpose of this paper is to study one of the "bad" cases, the triangular lattice, on which this symmetry between positive and negative J does not exist. It will be shown that there is no phase transition at any finite T if $J < 0$. To study the situation in more detail we will solve the problem with different coupling constants J_1, J_2, J_3 along different directions (see Fig. 1). By varying J_3 while leaving $J_1 = J_2$ constant we will be able to go continuously from the square lattice ($J_3 = 0$) to the triangular lattice ($J_3 = J_1 = J_2$) thus gaining considerable insight into the problem.

II. PARTITION FUNCTION

We consider the Hamiltonian

$$H = -\sum_{(i,j)} J_{ij}\,\sigma_i \sigma_j\,, \tag{1}$$

where $\sigma_i = \pm 1$, i, j are sites on a triangular lattice on which we use a set of coordinates x, y integers (Fig. 1), and the symbol (i, j) means that the summation is over all pairs of nearest neighbors. The coupling constants J_{ij} are J_1 if the bond ij is parallel to the x axis; J_2 if the bond ij is parallel to the y axis; J_3 if the bond ij is parallel to the lines $x + y = \text{const}$. The sign of J_1 can be changed by the transformation $\sigma_i \to (-1)^x \sigma_i$, and the same is true for J_2 with $\sigma_i \to (-1)^y \sigma_i$. We can therefore assume, without loss of generality, that both J_1 and J_2 are positive and study the cases $J_3 > 0$ (ferromagnetic) and $J_3 < 0$ (antiferromagnetic).

To find the partition function we adapt to the present situation a method due to Vdovichenko[8] and Feynman.[5] A detailed presentation of this method is found in Refs. 3–5. The partition function

$$Z = \sum_{\text{states}} \exp\left(\beta \sum_{(i,j)} J_{ij}\,\sigma_i \sigma_j\right) \tag{2}$$

can be written, using the identity

$$e^{\beta J_{ij}\sigma_i\sigma_j} = \cosh\beta J_{ij}\left[1 + (\tanh\beta J_{ij})\sigma_i\sigma_j\right], \tag{3}$$

as

$$\begin{aligned} Z &= (\cosh\beta J_1 \cosh\beta J_2 \cosh\beta J_3)^N \\ &\quad\times \sum_{\text{states}} \prod_{(i,j)} (1 + \sigma_i\sigma_j \tanh\beta J_{ij}) \\ &= (2 \cosh J_1 \cosh J_2 \cosh J_3)^N \\ &\quad\times \left\langle \prod_{(i,j)} (1 + \sigma_i \sigma_j \tanh\beta J_{ij}) \right\rangle, \end{aligned} \tag{4}$$

where N is the total number of sites and $\langle\ \rangle$ means average over all spin configurations. By expanding the product in (4) we obtain a diagrammatic expansion for Z in the usual way; for example, if a, b, c are three sites as shown in Fig. 2, the term

$$\langle \sigma_a \sigma_b \tanh\beta J_{ab} \sigma_b \sigma_c \tanh\beta J_{bc}\, \sigma_c \sigma_a \tanh\beta J_{ca} \rangle$$

is represented by the diagram shown on the same figure. Since

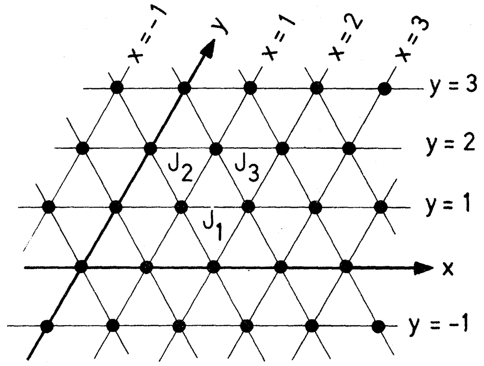

FIG. 1. Coordinates for the triangular Ising model. Two neighboring spins interact with a coupling constant which may be J_1, J_2, or J_3 according to the direction of the bond connecting them.

$$\langle \sigma_i^N \rangle = \begin{cases} 1, & n \text{ even} \\ 0, & n \text{ odd} \end{cases}, \tag{5}$$

the expansion of Z will only contain diagrams (linked or not) with an even number of lines emanating from each site. These are usually called "closed" diagrams.

The procedure we shall adopt consists in considering walks on the lattice which, starting from the origin, reach a site x, y in n steps and carry a weight calculated according to the following rules: (a) a factor $v_1 \equiv \tanh\beta J_1$ for each step parallel to the x axis; (b) a factor $v_2 \equiv \tanh\beta J_2$ for each step parallel to the y axis; (c) a factor $v_3 \equiv \tanh\beta J_3$ for each step parallel to the lines $x + y = \text{const}$; (d) a factor $e^{i\theta/2}$ for each turn by an angle $\theta = -\frac{2}{3}\pi, -\frac{1}{3}\pi, 0, \frac{1}{3}\pi, \frac{2}{3}\pi$; (e) a factor 0 for each turn by an angle π. For the only purpose of assigning an angle θ to the first step, we assume a "step 0" that led to the origin from the left.

As an illustration, the walk represented in Fig. 3 carries a weight

$$w = e^{i10\pi/12} v_1^3 v_2^3 v_3^2.$$

Let $A_n(x, y)$ be the sum of the amplitudes of all walks which reach x, y in exactly n steps, with the restriction that the last step must be in the positive x direction. Similarly, let $B_n(x, y)$, $C_n(x, y)$, $D_n(x, y)$, $F_n(x, y)$, $G_n(x, y)$ be the amplitudes with the last step taken as shown in Fig. 4. The following recurrence relations are a consequence of our rules:

$$\begin{aligned} A_{n+1}(x, y) = v_1[&A_n(x-1, y) + \bar{\epsilon} B_n(x-1, y) \\ &+ \bar{\epsilon}^2 C_n(x-1, y) + \epsilon^2 F_n(x-1, y) \\ &+ \epsilon G_n(x-1, y)], \\ B_{n+1}(x, y) = v_2[&\epsilon A_n(x, y-1) + B_n(x, y-1) \\ &+ \bar{\epsilon} C_n(x, y-1) + \bar{\epsilon}^2 D_n(x, y-1) \\ &+ \epsilon^2 G_n(x, y-1)], \\ &\vdots \end{aligned} \tag{6}$$

with $\epsilon \equiv e^{i\pi/6}$. We have indicated by dots the equations for C, D, F, and G, but the reader should have no difficulty in writing them out explicitly. Defining

$$A_n(x, y) \equiv (2\pi)^{-2} \int\int_0^{2\pi} d\xi\, d\eta\, \tilde{A}_n(\xi, \eta) e^{i(\xi x + \eta y)},$$

the first equation in (6) becomes

$$\tilde{A}_{n+1}(\xi, \eta) = v_1 e^{-i\xi}[\tilde{A}_n(\xi, \eta) + \bar{\epsilon}\tilde{B}_n(\xi, \eta) + \bar{\epsilon}^2 \tilde{C}_n(\xi, \eta) + \epsilon^2 \tilde{F}_n(\xi, \eta) + \epsilon \tilde{G}_n(\xi, \eta)], \tag{7}$$

and similarly for the other quantities. Collecting A, B, C, D, F, G into a column vector $\tilde{\underline{A}}$ we can write (7) in the more compact form

$$\tilde{\underline{A}}_{n+1} = \underline{M}\,\tilde{\underline{A}}_n, \tag{8}$$

with the matrix M given by

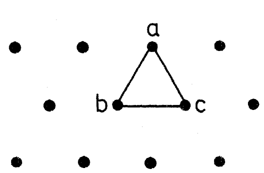

FIG. 2. Simplest diagram appearing in the expansion of Z.

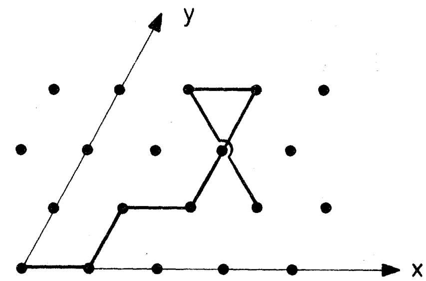

FIG. 3. Eight-step walk from the origin to site (3, 1).

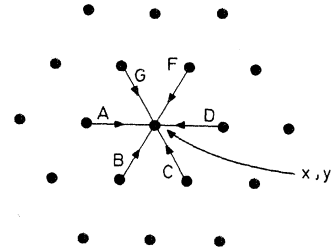

FIG. 4. Assignment of letters to the amplitudes for reaching site x, y from different directions.

$$M = \begin{bmatrix} v_1 e^{-i\xi} & 0 & 0 & 0 & 0 & 0 \\ 0 & v_2 e^{-i\eta} & 0 & 0 & 0 & 0 \\ 0 & 0 & v_3 e^{-i(\eta-\xi)} & 0 & 0 & 0 \\ 0 & 0 & 0 & v_1 e^{i\xi} & v_2 e^{i\eta} & 0 \\ 0 & 0 & 0 & 0 & 0 & v_3 e^{i(\eta-\xi)} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & \bar{\epsilon} & \bar{\epsilon}^2 & 0 & \epsilon^2 & \epsilon \\ \epsilon & 1 & \bar{\epsilon} & \bar{\epsilon}^2 & 0 & \epsilon^2 \\ \epsilon^2 & \epsilon & 1 & \bar{\epsilon} & \bar{\epsilon}^2 & 0 \\ 0 & \epsilon^2 & \epsilon & 1 & \bar{\epsilon} & \bar{\epsilon}^2 \\ \bar{\epsilon}^2 & 0 & \epsilon^2 & \epsilon & 1 & \bar{\epsilon} \\ \bar{\epsilon} & \bar{\epsilon}^2 & 0 & \epsilon^2 & \epsilon & 1 \end{bmatrix} . \tag{9}$$

Our convention about the step 0 provides the initial condition

$$\underline{\tilde{A}_0} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} . \tag{10}$$

The amplitude for returning to the origin in n steps, the last one being in the positive x direction, is, accordingly,

$$\begin{aligned} A_n(0, 0) &= (2\pi)^{-2} \int\int_0^{2\pi} d\xi\, d\eta\, \tilde{A}_n(\xi, \eta) \\ &= (2\pi)^{-2} \int\int_0^{2\pi} d\xi\, d\eta\, (\underline{M}^n)_{11} . \end{aligned} \tag{11}$$

We can now identify the last step with our hypothetical "step 0" so that our previous convention becomes superfluous. Equation (11) is then simply the weight assigned to the closed walks containing the origin and passing through this point at least once in the positive x direction. The weight of all closed n-step paths containing the origin with no restriction as to the direction of passage is, in analogy with (11)

$$Q_n(0, 0) = (2\pi)^{-2} \int \int_0^{2\pi} d\xi\, d\eta\, \mathrm{Tr}(\underline{M}^n) . \tag{12}$$

From this point on the argument is exactly as given in Refs. 3–5 (see also Sherman[9]) and need not be repeated. The final result is

$$\begin{aligned} \left\langle \prod_{(i,j)} (1 + \sigma_i \sigma_j \tanh\beta J_{ij}) \right\rangle &= \exp\left(-\frac{N}{2} \sum_{n=1}^{\infty} \frac{Q_n(0, 0)}{n} \right) \\ &= \exp\left(\frac{N}{2} \frac{1}{(2\pi)^2} \int \int_0^{2\pi} d\xi\, d\eta \right. \\ &\qquad \left. \times \ln\det(1 - \underline{M}) \right) , \end{aligned} \tag{13}$$

and since $Z = e^{-\beta F}$, we get from (4)

$$-(\beta F/N) = \ln 2 + \ln(\cosh\beta J_1 \cosh\beta J_2 \cosh\beta J_3) + \frac{1}{2} \frac{1}{(2\pi)^2} \int \int_0^{2\pi} d\xi\, d\eta \ln\det(1 - \underline{M}) . \tag{14}$$

From the explicit form of $\underline{M}$, Eq. (9), we find

$$\begin{aligned} \det(1 - \underline{M}) &= (1 + v_1^2)(1 + v_2^2)(1 + v_3^2) + 8 v_1 v_2 v_3 - 2 v_1 (1 - v_2^2)(1 - v_3^2) \cos\xi \\ &\quad - 2 v_2 (1 - v_1^2)(1 - v_3^2) \cos\eta - 2 v_3 (1 - v_1^2)(1 - v_2^2) \cos(\eta - \xi) \\ &= (\cosh\beta J_1 \cosh\beta J_2 \cosh\beta J_3)^{-2} [\cosh 2\beta J_1 \cosh 2\beta J_2 \cosh 2\beta J_3 + \sinh 2\beta J_1 \sinh 2\beta J_2 \sinh 2\beta J_3 \\ &\quad - \sinh 2\beta J_1 \cos\xi - \sinh 2\beta J_2 \cos\eta - \sinh 2\beta J_3 \cos(\eta - \xi)] , \end{aligned} \tag{15}$$

which, together with (14), constitutes the complete solution of the problem for arbitrary J_1, J_2, J_3.

III. CRITICAL TEMPERATURE

Nonanalytic behavior in F can occur only when

$$\det(1-\underline{M})=0\,. \tag{16}$$

This is therefore the condition for a critical point. Assuming first $J_1=J_2=J_3>0$, Eq. (15) reduces to

$$\det(1-\underline{M})=(1+v^2)^3+8v^3-2v(1-v^2)^2\times[\cos\xi+\cos\eta+\cos(\eta-\xi)]\,, \tag{17}$$

with a minimum at $\eta=\xi=0$,

$$\begin{aligned}\min[\det(1-\underline{M})]&=(1+v^2)^3+8v^3-6v(1-v^2)^2\\&=(1+v)^2(v^2-4v+1)^2\,.\end{aligned} \tag{18}$$

A zero occurs when $v^2-4v+1=0$, or

$$v=\tanh\beta_c J=2-\sqrt{3} \tag{19}$$

and we recapture here a known result.[6]

We consider next the case $J_1=J_2$ with a different value of J_3; we assume $J_3>0$. The minimum of $\det(1-\underline{M})$ still occurs for $\xi=\eta=0$. Calling $v_1=v_2=v;\ v_3=w$,

$$\begin{aligned}\min[\det(1-\underline{M})]&=(1+v^2)^2(1+w^2)+8v^2w\\&\quad-4v(1-v^2)(1-w^2)-2w(1-v^2)^2\\&=[w(v^2-2v-1)-(v^2+2v-1)]^2\,.\end{aligned} \tag{20}$$

The critical temperature is obtained from

$$w=\frac{v^2+2v-1}{v^2-2v-1}=1-\frac{4}{(1/v)+2-v}\,, \tag{21}$$

which can be solved numerically for T_c. The result is represented in Fig. 5.

Finally we consider the antiferromagnetic case $J_3<0$ while still holding $J_1=J_2$ for simplicity. If we consider

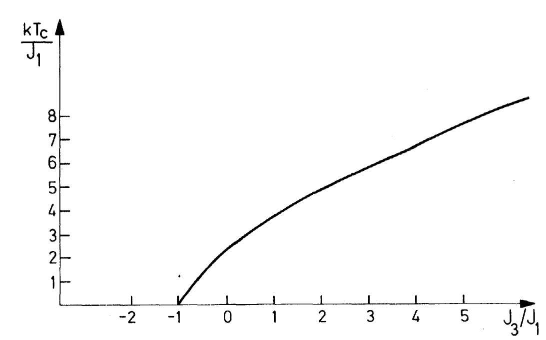

FIG. 5. Transition temperature as a function of J_3 for fixed $J_1=J_2$.

$$\begin{aligned}\det(1-\underline{M})&=(1+v^2)^2(1+w^2)+8v^2w\\&\quad-2v(1-v^2)(1-w^2)(\cos\xi+\cos\eta)\\&\quad-2w(1-v^2)^2\cos(\eta-\xi)\end{aligned} \tag{22}$$

as a function of ξ, η, there may be minima when

$$\begin{aligned}&2v(1-v^2)(1-w^2)\sin\xi-2w(1-v^2)^2\sin(\eta-\xi)=0\,,\\&2v(1-v^2)(1-w^2)\sin\eta+2w(1-v^2)^2\sin(\eta-\xi)=0\,.\end{aligned} \tag{23}$$

Disregarding solutions which are obvious maxima or saddle points we are left with two possibilities:

(a)

$$\xi=2\pi-\eta\,, \tag{24}$$

$$\cos\xi=\cos\eta=-\frac{1}{2}\frac{v(1-w^2)}{w(1-v^2)}\,, \tag{25}$$

$$\cos(\eta-\xi)=\frac{1}{2}\frac{v^2(1-w^2)^2}{w^2(1-v^2)^2}-1\,. \tag{26}$$

At this point

$$\begin{aligned}\det(1-\underline{M})&=(1+v^2)^2(1+w^2)+8v^2w\\&\quad+(1/w)v^2(1-w^2)^2+2w(1-v^2)^2\\&=(1+w)^2(1+v^2w)(1+v^2/w)\,.\end{aligned} \tag{27}$$

The only factor with a chance to vanish is the last one, but $w=-v^2$ is incompatible with $|\cos\xi|\leq 1$ in (25). We therefore must turn to the second possibility:

(b) $\xi=\eta=0$. But this will lead again to Eq. (21). We conclude that (21) is the necessary and sufficient condition for a critical point. To discuss its possible roots we have plotted in Fig. 6 the function

$$\phi\left(\frac{kT}{J_1}\right)=1-\frac{4}{1/v+2-v} \tag{28}$$

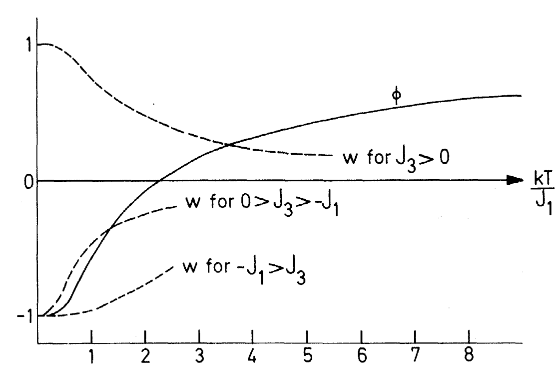

FIG. 6. Intersection of the full curve (ϕ) and the dashed curve (w) gives the root of Eq. (21) and thus the critical temperature. No phase transition occurs if $-J_1\geq J_3$.

as well as $w = \tanh\beta J_3$ for several possible values of J_3. If $J_3 > 0$, w starts at 1 for $T = 0$ and is a decreasing function. We obtain a transition temperature $T_c > 2.27 J_1$, bigger than for the square Ising model. For $0 > J_3 > -J_1$, w starts at -1 but remains above ϕ at low T; there is a critical temperature in the range $0 < T_c < 2.27 J_1$. Finally, for $J_3 < -J_1$ the two curves do not intersect, w remaining above ϕ for all $T > 0$; no phase transition occurs.

It is also easy to derive the asymptotic forms of the curve in Fig. 5 by appropriate series expansions in Eq. (21). We simply give the results

$$kT_c \simeq \frac{2}{\ln 2}(J_1 - |J_3|) \quad \text{if } J_3 \to -J_1 \text{ from above,} \tag{29}$$

and

$$kT_c \simeq \frac{2J_3}{\ln(kT_c/2J_1)} \quad \text{if } J_3 \to +\infty\,. \tag{30}$$

IV. DISCUSSION OF RESULTS

The behavior when $J_3 \simeq -J_1$ can be understood in the following way: As long as $J_3 > -J_1$, the ground-state energy per spin is $-2|J_1| + |J_3|$, corresponding to a configuration with all spins up. Consider a partition of the plane in two regions by a boundary like shown in Fig. 7. The line always follows the direction of the x or y axis. If all spins in one of the regions are reversed, the increase in energy is $2(J_1 - |J_3|)$ per unit length of the boundary. This is so because each step of the boundary cuts a J_1 and a J_3 bond. The entropy per unit length of the boundary is $k\ln 2$: After each step the boundary can be continued in two ways, straight ahead or turning by 60°. The ground state will be thermodynamically unstable against formation of such boundaries when their free energy of formation is negative:

$$F = E - TS = 2(J_1 - |J_3|) - kT\ln 2 < 0 \tag{31}$$

or

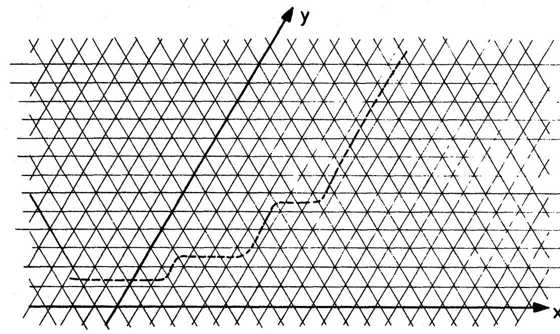

FIG. 7. Possible boundary between regions of opposite magnetization.

$$kT > 2(J_1 - |J_3|)/\ln 2 \tag{32}$$

in complete agreement with (29).

For $J_3 < -J_1$ the ground-state energy per spin is $-|J_3|$, exactly as if the system were composed of isolated antiferromagnetic chains in the J_3 direction. All spins in any one of these chains can be reversed with no change in the energy, so it is clear that no long-range order perpendicular to the chains can exist. As for long-range order along the chains, the usual argument about one-dimensional systems shows it to be impossible. In the absence of any kind of long-range order no cooperative phenomenon can exist.

Another interesting limit is $J_3 \to +\infty$. The system is then composed of unidimensional chains in the direction of J_3 with a weak interchain coupling provided by J_1 and J_2. Equation (30) can be written as

$$J_1 \simeq \tfrac{1}{2} kT_c\, e^{-2J_3/kT_c}\,. \tag{33}$$

A critical temperature kT_c of, say, 10% of J_3 requires $J_1 = 10^{-10} J_3$, while $kT_c = .05 J_3$ is achieved with an interchain coupling as low as $J_1 = 10^{-19} J_3$! The example clearly indicates that in such a situation any perturbative treatment, suggested by the small value of the interchain coupling, should be mistrusted.

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