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Second-order Phase Transitions in Triangular
Ising Models with Two- and Three-spin Interactions

by

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Abstract

For Ising models with pair and three-spin interactions on the triangular lattice the nature of the phase diagram in the temperature-field plane is studied. Second-order transitions are located by the interface method of Müller-Hartmann and Zittartz.

1. Introduction and model

The interest in the nature of phase transitions without the usual spin-reversal symmetry in zero field was considerably stimulated when Baxter and Wu¹ obtained the exact zero-field solution for the Ising model with three-spin interactions on the triangular lattice. This model is not in the same universality class as the nearest-neighbour ferromagnet² on the same lattice, since the specific heat critical index α has the value $\frac{2}{3}$ for the Baxter-Wu model and zero for nearest-neighbour interactions. Thus the natural question arises: What are the properties of systems with the general Hamiltonian

$$\mathcal{H} = J \sum_{(ij)} s_i s_j + J_3 \sum_{(ijk)} s_i s_j s_k - H \sum_i s_i, \quad (1)$$

incorporating the two known exact solutions^{1,2} as the special cases in which H and one of the coupling constants both are zero. Each interacting spin triplet (i,j,k) surrounds an elementary cell of the triangular lattice and (i,j) represents two nearest-neighbour sites.

Before taking up the problem of the critical properties of this generalized model (a problem to which conflicting answers^{3,4,5} have been given), one would like to have an over-all view of the phase diagrams of the different spin systems. In particular one would wish to know the complete phase diagram of the Baxter-Wu model in non-zero magnetic fields. The Hamiltonian (1) contains just one non-trivial parameter, viz. the ratio J/J_3 , or equivalently

$$R = \frac{J}{J_3 + |J|}, \quad (2)$$

and it would be of interest to see how the general phase diagrams

interpolate between the ferromagnetic transition² in zero field ($R=-1$) via the Baxter-Wu transition ($R=0$) to the fairly well-established antiferromagnetic transition^{6,7,8} in non-zero magnetic field ($R=1$).

For ferromagnetic pair interactions ($J < 0$) the phase diagram for the Hamiltonian (1) has been calculated in a mean-field treatment corresponding to a three-sublattice structure.⁹ The results are sketched in Fig.1. Mean-field theory is known¹⁰, however, to yield topologically incorrect phase diagrams in certain cases. And it fails in a qualitative way at least for one special case of our Hamiltonian, viz. the triangular antiferromagnet¹¹ ($R=1$).

Fig. 1. The phase diagram for the Hamiltonian (1) in the mean-field approximation (Ref.9). The pair interaction is ferromagnetic. The field is given in units of $|J| + J_3$, the temperature in units of $(|J| + J_3)/k$. In the closed regions the sublattice magnetizations are unequal. All transitions are first-order.

We use here another approach, the interface method¹². This method, for two-dimensional systems comparable in simplicity^{12,13,7} with the mean-field treatment, yields closed-form expressions for phase boundaries. For the square lattice antiferromagnet¹² the results are qualitatively correct and quantitatively reasonably accurate¹⁰. And for the triangular antiferromagnet the interface method yields⁷, in contradistinction to mean-field and mean-field-like treatments, the qualitatively correct phase diagram.

The interface method is limited in that it only locates second-order transitions. With the knowledge of the exact zero-temperature behaviour (section 2), we are, however, able to construct a consistent picture of the structure of the phase diagrams for different interaction strengths, even if the detailed description of the first-order transition lines is missing.

2. $T=0$

We will take $J_3 \geq 0$. This involves no loss of generality, since replacing J_3 by $-J_3$ in (1) is equivalent to reversing all spins as well as the external magnetic field. Hence the partition function is invariant under reversal of the odd couplings, $Z(J, -J_3, H) = Z(J, J_3, -H)$.

The Hamiltonian (1) may be considered as a sum of contributions $e(s_1 s_2 s_3)$ from the elementary triangular faces on the lattice. The four non-equivalent configurations of the three spins s_1, s_2 and s_3 at the vertices of a triangle have energies

$$e(+++) = \frac{3}{2}J + J_3 - \frac{1}{2}H, \quad (2a)$$

$$e(++-) = -\frac{1}{2}J - J_3 - \frac{1}{6}H, \quad (2b)$$

$$e(+--) = -\frac{1}{2}J + J_3 + \frac{1}{6}H, \quad (2c)$$

$$e(---) = \frac{3}{2}J - J_3 + \frac{1}{2}H. \quad (2d)$$

Since each of these four cell configurations can be repeated consistently over the lattice, the ground state of the spin system is found by minimizing the energy expressions (2) for the four basic spin configurations.

The result is conveniently summarized in Fig. 2. We see that for strong ferromagnetic interactions,

$$J \leq -\frac{2}{3}J_3, \quad (3)$$

only one zero-temperature transition occurs, otherwise at least two transitions are present at $T=0$. It is natural to predict that the transition in the range (3), i.e. $-1 \leq R \leq -\frac{2}{3}$, is a first-order transition similar to the ferromagnetic transition at $R=-1$.

Fig. 2. Ground-state configuration for the Hamiltonian (1). The transition lines are given by $H=6J+6J_3$ (L_1), $H=-6J_3$ (L_2), $H=-6J+6J_3$ (L_3), $H=-3J$ (L_4) and $H=2J_3$ (L_5). Three different ground states can coexist for $J=-\frac{2}{3}J_3$, $H=2J_3$, and for $J=2J_3$, $H=-6J_3$.

3. Critical states

By the interface method for a two-dimensional problem one undertakes a determination of the excess free energy F_s associated with an interface, by setting up a one-dimensional transfer matrix problem along the interface¹².

Critical lines or points result from setting

$$F_s(H,T) = 0 \quad (4)$$

The interface in question is a division line between homogeneous regions of ground-state configurations. The method has been applied to antiferromagnetic situations where one has doubly degenerate ground states, both on the square lattice¹² and on the triangular lattice¹³. The present authors utilized it for the triangular antiferromagnet⁷ with triply degenerate ground states. In the present case the ground states $(++-)$ and $(+--)$ are also triply degenerate since the minority spins may be situated on any of the three sublattices. The present calculation will, therefore, follow similar lines as in Ref.7, to which we refer for more details.

Consider first the interface between two regions each consisting of one of three degenerate $(++-)$ -states. The situation is shown in Fig.3 in which the triangular lattice is conveniently drawn in a deformed version.

In Fig.3 a horizontal reference interface is drawn. If we extend the lower phase upwards by turning a certain number n_i of spins in the i 'th column, the new displaced interface can be described by the set $\{n_i\}$ of integers, with the convention that negative n_i 's correspond to lowering the interface. Denoting the energy of the interface configuration $\{n_i\}$, relative to the standard interface, by $E(\{n_i\})$, we have

$$E(\{n_i \pm 2\}) = E(\{n_i\}) \quad (5)$$

Fig.3. The reference interface $\{0,0,0,0,0,0\}$ between two $(++-)$ - phases.

because the natural periodicity of three lattice units corresponds to turning two spins in every column.

One would rather know the excess energy $\Delta E(\{n_i\})$ relative to a homogeneous region with no interface, since the excess free energy F_s is given by

$$\exp(-\beta F_s) = \sum_{\{n_i\}} \exp(-\beta \Delta E) . \quad (6)$$

The difference between ΔE and E is simply the energy cost for creating the reference configuration, in this case

$$\Delta E(\{n_i\}) - E(\{n_i\}) = N(\frac{4}{3}J + \frac{8}{3}J_s) , \quad (7)$$

where N is the number of columns.

Since the Hamiltonian (1) contains no interactions that act beyond nearest-neighbour columns, the energy expression $E(\{n_i\})$ will be of the form

$$E(\{n_i\}) = E_1(n_1, n_2) + E_2(n_2, n_3) + E_3(n_3, n_4) + E_1(n_4, n_5) + E_2(n_5, n_6) + \dots \quad (8)$$

The three different types of intercolumn energy expressions turn out to be

$$E_1(n, m) = [2|n-m| + (-1)^n - (-1)^m]J + [4|n-m| - (-1)^n + (-1)^m]J_3 + \frac{1}{2}[(-1)^m - (-1)^n]H \quad (9a)$$

$$E_2(n, m) = [2|n-m| + (-1)^m - (-1)^n]J + [4|n-m| + (-1)^n - (-1)^m]J_3 + \frac{1}{2}[(-1)^n - (-1)^m]H \quad (9b)$$

$$E_3(n, m) = [2|n-m+1| - 4 + (-1)^n + (-1)^m]J + [4|n-m+1| - 2 - (-1)^n - (-1)^m]J_3 - \frac{1}{2}[(-1)^n + (-1)^m - 2]H \quad (9c)$$

By convention the magnetic field energy is shared equally between the left-hand and the right-hand intercolumn energy expressions.

The free energy is now determined by the maximum eigenvalue of the product of the three corresponding transfer matrices $T_{nm} = \exp[-\beta E(n, m)]$. By the periodicity (5) the problem is reduced to an eigenvalue problem for the product of the three 2×2 matrices⁷ ($n=1, 2, 3$)

$$\left(t_n \right)_{ik} = \sum_{m=-\infty}^{+\infty} \left(T_n \right)_{i, k+2m} \quad (10)$$

It is straightforward to determine the explicit form of these reduced

matrices. We find

$$t_1 = \begin{pmatrix} \cosh(2K+4P) & e^{-2K+2P+h} \\ e^{2K-2P-h} & \cosh(2K+4P) \end{pmatrix} \frac{1}{\sinh(2K+4P)} , \quad (11)$$

with

$$K=J/kT , \quad P=J_3/kT \quad \text{and} \quad h=H/kT . \quad (12)$$

Moreover,

$$t_2 = \tilde{t}_1 , \quad (13)$$

the transpose of t_1 ; and t_3 can also be expressed in terms of t_1 :

$$t_3 = e^{4K+2P-h} t_1 \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} . \quad (14)$$

The series (10) converges as long as $K > -2P$, which covers the whole range in which our $(++-)$ ground state occurs (Fig.2).

By (5) and (7) the free energy $F_S(H,T)$ connected with the interface equals, for large N ,

$$F_S(H,T)/N = -\frac{4}{3}K - \frac{8}{3}P + \frac{1}{3} \ln \lambda ,$$

with λ the maximum eigenvalue of the product $T_1 T_2 T_3$, i.e. of $t_1 t_2 t_3$. Thus F_S vanishes, eq.(4) , for $\lambda = \exp(4K+8P)$. One finds from this the following condition for criticality

$$2 \cosh(2h-6K) = \cosh^3(2K+4P) - 3 \cosh(2K+4P) \quad (15)$$

The zero-temperature behaviour corresponds to large coupling constants, and one sees that for $T \rightarrow 0$ the critical field must

satisfy $|2h-6K|=3(2K+4P)$, i.e. $h=6K+6P$ or $-6K$.

The field range

$$-6J_3 \leq H \leq 6J+6J_3 \quad (16)$$

covered by the critical line (15), corresponds for $-\frac{2}{3} \leq R \leq 1$ precisely to the field range for which the present ground state occurs. For the remaining range $-\frac{2}{3} \leq R \leq \frac{2}{3}$, where the ground state changes from $(++-)$ to $(---)$ with decreasing field, the $(++-)$ ground state with which we are concerned now, exists only in a subrange of (16), viz. for

$$-3J \leq H \leq 6J+6J_3 \quad (17)$$

By specializing to the Baxter-Wu case $J=0$ we see clearly that what happens is that the first-order transition at $H=0$ intervenes (Fig.4). The question of the critical end point of the first-order transition line will be discussed below.

Fig. 4. Phase diagram of the Baxter-Wu model.

The second-order transition is described by
 $2 \cosh 2h = \cosh^3 4P - 3 \cosh 4P$.

Let us now turn to the other triply degenerate ground state, $(+--)$, which is only present in the antiferromagnetic region. Configurations for this case may be recovered by spin reversal from configurations in the calculation we have just completed. It follows

that in this case the equation for criticality is obtained from (15) by reversing the sign of the odd couplings, i.e.

$$2 \cosh(2h+6K) = \cosh^3(2K-4P) - 3 \cosh(2K-4P) \quad (18)$$

The series (10) converges in this case only when $K > 2P$, i.e. precisely in the range where the $(+--)$ ground state occurs. The field range covered by (18) is

$$-6J + 6J_3 \leq H \leq -6J_3, \quad (19)$$

equal to the field range of the $(+--)$ ground state. Thus the ground-state transitions lines are identified as end points of second-order transitions in this case.

Consequently no first-order transitions is expected when the pair interaction is sufficiently antiferromagnetic, more precisely when $J > 2J_3$.

For $J > 2J_3$ the second-order lines (15) and (18) form two lobes in the field-temperature plane. For pure antiferromagnetic pair interactions the lobes are symmetrically placed. Mixing in more and more three-spin coupling into the interaction, the $(++-)$ -lobe increases and the $(+--)$ -lobe decreases in size until the latter disappears when J_3 reaches the value $\frac{1}{2}J$. (See Fig.6.)

Two of the triply degenerate ground states of either kind can coexist in a non-zero field range. The situation is different for any other pair of phases, $(+++)$ and $(---)$, say. They coexist only at one definite field value, as shown in Fig.2. By the interface method one may find an expression for the boundary tension σ for this value of the field and consequently obtain the critical temperature for which σ vanishes. The critical field will thus necessarily be the same as the field for which the ground-state transition occurs, $H_c(T_c) = H_c(0)$. No information about the critical field for intermediate temperatures

$0 < T < T_c$ is obtainable by the interface method.

Let us now work out the interface-method predictions for these critical points. The ferromagnetic transition between the ground states $(+++)$ and $(---)$ yields the simplest situation. In this case all intercolumn energy expressions are identical and equal to

$$E(n,m) = 2J - 4|n-m+\frac{1}{2}|J. \quad (20)$$

We have assumed that the upper phase is $(+++)$, and have used that $H=2J_3$ along the ground-state transition line L_5 in Fig.2. Since the transfer matrix $T(m,n) = \exp[-\beta E(n,m)]$ is of the form $T(m-n)$, the partition function equals λ^N , with

$$\lambda = \sum_{m=-\infty}^{+\infty} \exp(4K|n-m+\frac{1}{2}|-2K) = \frac{2}{1-e^{-4K}} \quad (21)$$

The energy cost in creating the reference interface is $-4NJ = 4|J|N$, and consequently we find the boundary tension $\sigma = F_s/N$ to be

$$\sigma = -4J - kT \ln[2/(1-e^{-4K})], \quad (22)$$

which vanishes for

$$T_c = 4|J|/\ln 3. \quad (23)$$

This result may be checked for pure ferromagnetic interactions ($J_3=0$). The exact critical temperature is known², and is precisely (23)! Equation (23) implies that the Curie temperature is not influenced by the presence of three-spin interactions, as long as $J_3 < \frac{3}{2}|J|$.

The only ground-state transition line not discussed so far is L_4 in Fig.2. By the evidence from the Baxter-Wu case we expect this to be the zero-temperature end-point of a first-order transition. We consider now the interface between the $(---)$ -phase and one of the $(++-)$ -phases. It is clear from Fig.5 that it is necessary to expend

an energy

$$\frac{2}{3}N[e(++-)-e(---)] = (-\frac{4}{3}J+\frac{8}{3}J_3)N \quad (24)$$

to create a reference interface of column width N . We need once more three different intercolumn energy expressions for a general (non-overhanging) interface. Using $H=-3J$ we find

$$E_1(n,m)=(4J_3-2J)|n-m|+(J_3-\frac{1}{2}J)[(-1)^m-(-1)^n] , \quad (25a)$$

$$E_2(n,m)=E_1(m,n) , \quad (25b)$$

and

$$E_3(n,m)=E_1(n,m-1)+J-2J_3 . \quad (25c)$$

Note that these energy expressions can be obtained from the corresponding previous expressions (9) by replacing J by $-J$ and H by $-3J$ in (9). Moreover, we see that the same replacement in eq.(7) reproduces the corresponding expression (24) for the energy cost of the reference interface. Consequently we obtain without any further calculation the condition for criticality in the present case by the same substitution in equation (15), with the result

$$2=\cosh^3(4P-2K)-3 \cosh(4P-2K) \quad (26)$$

The solution is $\cosh(4P-2K)=2$ or

$$T_c=(4J_3-2J)/k\ln(2+\sqrt{3}) . \quad (27)$$

Note first that the critical temperature (27) vanishes for $J=2J_3$, which is precisely the end-point of the region where the first-order transition occurs. Secondly, for pure triplet interactions ($J=0$) we see that the zero-field endpoint of the second-order transition (15),

$$2 \cosh 2h=\cosh^3 4P-3 \cosh 4P \quad (28)$$

Fig. 5. The reference interface between $(---)$ -phase and a $(++-)$ -phase. The energy cost in creating this interface is associated with the shaded triangular faces.

is equal to the critical temperature (27). For the Baxter-Wu model the end-points of the first-order and second-order transition thus coincide in the present approximation. This feature, which may well be exact, is not present in the mean-field result (Fig.1).

Finally, we mention that one can study the interface between one of the $(++-)$ ground states and the $(+++)$ state, i.e. at a field $H=6J+6J_3$ (line L_1 in Fig.2), and similar a $(++-)-(+-)$ interface along L_2 or a $(+-)-(---)$ interface along L_3 . In all these cases we find $T_c=0$, as should be.

4. Summary and conclusion

A general conclusion is that the transition lines L_1 , L_2 and L_3 in the zero-temperature diagram (Fig.2) are connected to second-order transitions. The two other zero-temperature transitions L_4 and L_5 are considered to belong to first-order transitions. The over-all picture is best shown by a sequence of characteristic phase diagrams, as in Fig.6.

The second-order transitions are described by the closed-form expression (15) and (18):

Fig. 6. Phase diagram in the temperature-field plane for varying interaction ratios R . Second-order boundaries are shown with solid lines. Filled circles show the interface-method predictions for critical end-points of first-order transitions. The first-order transitions are arbitrarily drawn parallel to the temperature axis with dashed or dotted lines. (Boundaries of regions with different sublattice magnetizations are dashed). Fields are measured in units of $|J|+J_3$, temperatures in units of $(|J|+J_3)/k$.

$$2 \cosh(2h \pm 6K) = \cosh^3(2K \mp 4P) - 3 \cosh(2K \mp 4P) \quad (30)$$

These results are exact at zero temperature, but how good are they at finite temperatures? For $J_3=0$ the result may be compared with Monte-Carlo calculations. The agreement is fair, with the prediction for the critical temperature somewhat low when the magnetic field is small and somewhat high for stronger fields. We refer to Ref.7 for details of this comparison. For $J=0$ the critical temperature (27), numerical $T_c \approx 3.04 J_3/k$, may be compared with the exact critical temperature $T_c = 2J_3/k \ln(1+\sqrt{2}) \approx 2.27 J_3/k$.

The zero-temperature slope of our transition lines (30) can also be compared with exact results. We find from (30) that at the endpoints $H=6J_3 \pm 6J$

$$\left(\frac{\partial kT}{\partial H} \right)_{T=0} = \mp \frac{2}{\ln 8} = \mp 0.96, \quad (31)$$

independent of the interactions.

The exact result for the slope can be found by taking the zero-temperature limit of the corresponding lattice gas. Introducing

$$\epsilon_i = \frac{1}{2}(1 \pm s_i), \quad (32)$$

the presence of a particle ($\epsilon=1$) is associated with a spin up(down) for the upper (lower) sign.

The partition function for the Hamiltonian (1), transforms into the grand partition function for a lattice gas:

$$Z = \sum_{\{\epsilon_i=0,1\}} e^{-\beta H} = \sum_{\{\epsilon_i=0,1\}} \exp \left[-(4K \mp 8P) \sum_{(ij)} \epsilon_i \epsilon_j \mp 8P \sum_{(ijk)} \epsilon_i \epsilon_j \epsilon_k \right] z^{\sum_i \epsilon_i}, \quad (33)$$

with

$$z = e^{\pm 2h \mp 12P + 12K} \quad (34)$$

omitting an uninteresting constant.

We will now study the $T \rightarrow 0$ limit for this partition function. Take first the upper signs. For $J > 0$ and $J_3 < \frac{1}{2}J$ the coefficients of both the pair and triplet interaction terms in (33) are positive. In the zero-temperature limit (33) thus describes a lattice gas with nearest-neighbour exclusion, a hard-hexagon lattice gas. Baxter¹⁴ has shown that this lattice gas has a phase transition at a critical fugacity $z_c = \frac{11}{2} + \frac{5}{2}\sqrt{5}$. Translating back to the spin system we see that the transition is described by

$$H - 6J_3 + 6J = \frac{1}{2}kT \ln z_c \quad (35)$$

near $T=0$.

For the lower signs in (33) we rewrite the Hamiltonian in (33) as a sum over the triangular faces,

$$Z = \sum_{\{\epsilon_i=0,1\}} \exp \left[-\beta \sum_{(ijk)} \hat{e}(\epsilon_i, \epsilon_j, \epsilon_k) \right] z^{\sum \epsilon_i} \quad (36)$$

with

$$\hat{e}(\epsilon_i, \epsilon_j, \epsilon_k) = -8J_3 \epsilon_i \epsilon_j \epsilon_k + (2J + 4J_3)(\epsilon_i \epsilon_j + \epsilon_i \epsilon_k + \epsilon_j \epsilon_k)$$

Since $\hat{e}(\epsilon_i, \epsilon_j, \epsilon_k)$ vanishes if more than one ϵ is zero, while

$$\hat{e}(1,1,1) = 4J_3 + 6J \text{ and } \hat{e}(1,1,0) = 4J_3 + 2J, \quad (37)$$

we see that for $J > -\frac{2}{3}J_3$ we once more have nearest-neighbour exclusion in the $T \rightarrow 0$ limit. This leads to

$$-H + 6J_3 + 6J = \frac{1}{2}kT \ln z_c, \quad (38)$$

instead of (35), for the magnetic transition near zero temperature.

We thus have the exact result for the zero-temperature slope

$$\left(\frac{\partial kT}{\partial H} \right)_{T=0} = \mp \frac{1}{2} \ln \left(\frac{11}{2} + \frac{5}{2}\sqrt{5} \right). \quad (39)$$

The upper sign is valid along the line L_1 in Fig.2, i.e. near

$H=6J+6J_3$, the lower sign along L_3 , i.e. near $H=6J_3-6J$.

The regions of validity derived above correspond precisely to those ratios of interactions for which the two second-order transitions (30) occur.

Comparing the result (31) of the interface method with the exact result (39) we see that the numerical value (31) is somewhat high, viz. 0,96 compared to the exact value of approximately 0,83. We reproduce the exact result that the zero-temperature slope is completely independent of the interaction strengths.

The mean-field results⁹ (Fig.1) are not in qualitative agreement with the present results since our second-order transition is represented by a first-order transition. (The jump in magnetization across this mean-field transition is in general rather small, however⁹). One can also see from Fig.1 that the zero-temperature slope (for the Baxter-Wu model, say) does not even have the correct sign in mean-field theory. It would be very interesting if one could improve the mean-field theory also for the description of the genuine first-order transitions. A treatment based upon Baxter's variational approximations¹⁵ seems feasible¹⁶.

In conclusion, we have presented the interface-method treatment of Ising spin systems on the triangular lattice with two- and three-spin interactions. Our main results are approximate closed-form expressions for the second-order transitions, together with qualitative predictions of the structure of the phase diagram for all ratios of the interactions, ranging from the ferromagnet via the Baxter-Wu model to the antiferromagnet.

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