Tricritical Properties of Antiferromagnetic Ising Model on the Square Lattice

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Abstract

The Ising square lattice model with nearest-neighbor (nn) interactions \((J_1)\) is one of the few exactly solvable models \([1]\). Adding next-nearest-neighbor (nnn) interactions \((J_2)\) or a magnetic field (or both) leads to the non solvability of the model and only some approximate solutions are possible. In this brief report we will review some results obtained within effective field theory. We will show that besides second-order transitions there are also lines of first-order transitions and the coordinates of tricritical points are calculated.

The Hamiltonian of the Ising model with competing antiferromagnetic (AF) interactions between nn \((J_1 < 0)\) and nnn \((J_2 < 0)\) spins in zero external field is

\[
H = -J_1 \sum_{nn} \sigma_i \sigma_j - J_2 \sum_{nnn} \sigma_i \sigma_j, \tag{1}
\]

where classical spin variable \(\sigma_i\) can acquire two values \(\pm 1\), and summations runs over corresponding pairs of interacting spins. For better visualization the geometrical structure of the model is depicted on the Fig. 1. From an experimental point of view, such model could describe quasi-two-dimensional anisotropic AF like K\(_2\)CoF\(_4\) compound at least within a fair approximation. Since the existence of nnn interactions and the magnetic field may give rise to other phases with different types of phase transitions and multicritical points, we restrict ourselves to the AF interactions with zero magnetic field. In such model it is also expected presence of so-called superantiferromagnetic (SAF) - striped phase.

Our main aim is to determine the phase diagram in the parameter space \((\alpha, t)\) (defined below, see 5) using an effective field theory based on succesive use of one-, two-, and four-spin clusters. Used approach is based on the differential operator technique \([2]\) introduced into exact Ising spin identities and has already been successfully applied to a variety of spin-\(\frac{1}{2}\) and higher spin problems. Of course, the effective field calculation cannot give any precise information about the value of critical exponents. The starting point of the effective field theory is
the so-called set of correlation identities. By standard procedure involving use of van der Waerden identity and truncation procedure it is possible to get closed set of equations for spin-correlations functions. We will restrict ourselves to the simplest possible truncation scheme

\[ \langle \sigma_i \cdot \sigma_j \cdots \rangle \approx \langle \sigma_i \rangle \cdot \langle \sigma_j \rangle \cdots \quad (i \neq j \neq \cdots). \tag{2} \]

In order to take into account effects of frustration within the present effective-field theory, it is necessary to consider at least two-spin cluster. By relatively straightforward calculation the normalized staggered magnetization \( m_s \) associated with the antiferromagnetic two-spin cluster is given by

\[
m_s = \left[ A_x(1)A_y(2) + B_x(1)B_y(2) + m_B \left( A_x(1)B_y(2) + A_y(2)B_x(1) \right) \right]^2 \times \left[ A_y(1)A_x(2) + B_y(1)B_x(2) + m_A \left( A_y(1)B_x(2) + A_x(2)B_y(1) \right) \right]^2 \times \left( A_x(1) + m_B B_x(1) \right) \left( A_y(1) + m_A B_y(1) \right) \times \left[ \left( A_x(2) + m_A B_x(2) \right) \left( A_y(2) + m_B B_y(2) \right) \right]^2 f_s(x, y) \bigg|_{x=0, y=0}, \tag{3} \]

where \( m_s = (m_A - m_B)/2 \) represents an order parameter for AF phase, \( A_\mu(\nu) = \cosh(J_\nu D_\mu), B_\mu(\nu) = \sinh(J_\nu D_\mu) \) \( (\nu = 1, 2) \), \( D_\mu \equiv \partial/\partial \mu \). The function \( f_s(x, y) \) is defined as follows

\[
f_s(x, y) = \frac{\sinh \beta(x - y)}{\cosh \beta(x - y) + e^{2\beta J_1} \cosh \beta(x + y)}, \tag{4} \]

where \( \beta = 1/k_B T \) is reduced inverse temperature. Equation of state is quite superior to that obtained from the standard mean-field theory, since in
the present framework relations like $(s_α g)^{2r} = 1$ and $(s_α g)^{2r+1} = s_α g$, for all $r$, are taken exactly into account through the van der Waerden identity, $\exp(a s_α g) = \cosh(a) + s_α g \sinh(a)$. On the other hand in the usual molecular-field theory not only multi-spin correlations are neglected but so are self-correlations of spin variables.

It is convenient to introduce dimensionless effective parameters $t$ and $\alpha$ by the following relations

$$\alpha = \frac{J_2}{|J_1|}, \quad t = \frac{1}{\beta |J_1|}. \quad (5)$$

Since for the antiferromagnetic $J_1 - J_2$ model at zero magnetic field the following symmetry $m_s \leftrightarrow -m_s$ for the staggered magnetization holds, Eq. (3) can be recast in the form

$$m_s = \sum_{n=0}^{4} K_{2n+1}^{AF} m_s^{2n+1}, \quad (6)$$

where only the odd coefficients $K_{2n+1}^{AF}$ are present. These coefficients depend on $t$ and $\alpha$ and can be easily calculated using symbolic calculations by direct employ of translational formula

$$\exp(\lambda D_x + \gamma D_y) f_s(x,y) = f_s(x+\lambda, y+\gamma). \quad (7)$$

Because the final expressions for coefficients $K_{2n+1}^{AF}$ are quite lengthy, their explicit form is omitted. We note also that in obtaining Eq. (6) we have made use of the fact that $f_s(x,y) = -f_s(-x,-y)$ and therefore only odd differential operator functions remain.

In order to determine the phase diagram of the antiferromagnetic $J_1 - J_2$ model, we should solve Eq. (6) for a given value of the frustration parameter $\alpha$ and look for the temperature at which the magnetization (order parameter) $m_s$ goes to zero. However, for a some value of $\alpha$, the order parameter goes to zero discontinuously, accordingly the transition becomes first order. To analyze such transition, one needs to calculate the free energy for the antiferromagnetic and paramagnetic phases and to find a point of intersection. Because the expression for the free energy in this effective-field theory does not exist, it will be extrapolated with the help of the relation for the equilibrium value of the order parameter (6) as follows (4):

$$F^{AF}(t, \alpha, m) = F_0(t, \alpha) + \frac{1}{2} \left( 1 - \sum_{n=0}^{4} \frac{K_{2n+1}^{AF}}{n+1} m_s^{2n} \right) m_s^2, \quad (8)$$

where $F_0(t, \alpha)$ is a free energy of the disordered (paramagnetic) phase and $m$ is the order parameter which takes the value $m_s$ at thermodynamic equilibrium. We note that relation (8) corresponds to a Landau free energy expansion in the order parameter truncated in the $m^{10}$ term.

Thus the equilibrium magnetization is the value of the order parameter, which minimizes the free energy given by the Eq. (8). Using the equilibrium condition

$$\left. \frac{\partial F^{AF}(T, \alpha, m)}{\partial m} \right|_{m=m_s} = 0, \quad (9)$$
we recover the Eq. (6) for the equilibrium magnetization. Then a critical temperature and a tricritical point, at which the phase transition changes from second order to first order, are determined as follows: (i) second-order transition line when $1 - K_{1}^{AF} = 0$ and $K_{3}^{AF} < 0$, and (ii) tricritical point when $1 - K_{1}^{AF} = 0$, $K_{3}^{AF} = 0$, if $K_{5}^{AF} < 0$. It is worth noticing that if we use this relations to obtain the critical and tricritical points, the results coincide with those obtained from Eq. (6). We believe that this justifies our procedure. However, the first-order phase transition line is evaluated by solving simultaneously two transcendental equations, namely $[\text{9}]$ and $F^{AF}(t, \alpha, m) = F_{0}(t, \alpha)$, which corresponds to the point of intersection of the free energy antiferromagnetic and paramagnetic phases.

Analogous procedure could also be performed for the superantiferromagnetic phase. After some algebraic manipulations it can be shown that the corresponding equation of state is

$$m_{s} = \left[ A_{x}(1)A_{y}(2) + B_{x}(1)B_{y}(2) + m_{A}\left( A_{x}(1)B_{y}(2) + A_{y}(2)B_{x}(1) \right) \right]^{2}$$

$$\times \left[ A_{y}(1)A_{x}(2) + B_{y}(1)B_{x}(2) + m_{B}\left( A_{y}(1)B_{x}(2) + A_{x}(2)B_{y}(1) \right) \right]^{2}$$

$$\times \left( A_{x}(1) + m_{B}B_{x}(1) \right) \left( A_{y}(1) + m_{A}B_{y}(1) \right)$$

$$\times \left[ \left( A_{x}(2) + m_{B}B_{x}(2) \right) \left( A_{y}(2) + m_{A}B_{y}(2) \right) \right]^{2} f_{s}(x, y) \bigg|_{x=0, y=0}.$$  

(10)

Thus, using of the same sort of approximate scheme as before, we obtain numerically the second- and first-order transition lines including the tricritical point between the superantiferromagnetic and paramagnetic phases.

One can of course imagine a continuation of the this process with considering larger and larger clusters. As a consequence better results for thermodynamic properties are expected. Because of natural limitations of computer power one cannot expect to solve this problem exactly (which would basically correspond to the infinite cluster) within the used method. Therefore, the next step is a cluster with four spins containing the information of the lattice topology. Using the same procedure as before for the two-spin cluster, one determines the second- and first-order transition line including tricritical point between the ordered (antiferromagnetic or superantiferromagnetic) and paramagnetic phases.
Let’s discuss basic features of the phase diagram. To get some insight into the problem we start with analysis of the ground state \((t = 0)\). The expected ordered states are graphically represented on the Fig. 2 and their energies are

\[
\frac{E_{SAF}}{N|J_1|} = 2\alpha, \quad \frac{E_{AF}}{N|J_1|} = -2(1 + \alpha).
\]  

By direct comparison we see, that for \(\alpha = -0.5\) there should be a phase transition from the AF phase to the SAF phase. Next by numerical analysis of equations (3) and (10) we were able to obtain second order transition lines between AF and para phase and also between SAF and para phase. Because of lack of space we will present here only results for the former case, which is depicted on the Fig. 3. As can be readily seen all used approximations lead to the prediction of existence of tricritical point. We obtained the similar picture also for the superantiferromagnetic-paramagnetic transition. To have more quantitative comparison we have listed coordinates for the tricritical points in the Tab. 1. Note also critical temperatures \(t_c\) for the case \(\alpha = 0\). The relative decreasing of the critical temperature is in agreement with the exact value \(t_{c,exact} = 2.2692\) for the given lattice [5].

Effective field theory doesn’t capture fluctuations in order parameter. It is well known that fluctuations are greatly pronounced in the critical region. Actually in some cases such fluctuations could lead to change 1-order phase transition into 2-order phase transition as is e.g. the case for random Ising model [6]. Such possibility could not be excluded by the effective field theory. Therefore more sophisticated methods are needed, such as Monte Carlo simulations [7, 8]. This method however have its own deficiencies such as sign problem in the region \(\alpha \approx -0.5\). Our next steps will be in automatization of algorithms to deal with \(N^2\)-site cluster approximation \((N = 3, 4, \ldots)\) and in comparison of obtained results with Monte Carlo simulations.
|                | 1-site | 2-site | 4-site |
|----------------|--------|--------|--------|
| $t_{tcp}^{AF}$ | 1.7002 | 1.3720 | 1.3066 |
| $\alpha_{TCP}^{AF}$ | −0.2383 | −0.2973 | −0.3070 |
| $t_{tcp}^{SAF}$ | 3.2207 | 2.2594 | 2.4619 |
| $\alpha_{tcp}^{SAF}$ | −1.3276 | −0.9991 | −1.0387 |
| $t_{cp}$        | 3.0898 | 3.0250 | 2.9197 |

Table 1: Coordinates of tricritical points and critical points for $\alpha = 0$ in various approximations.

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