The phase diagram for Potts model with competing ternary and binary interactions on a Cayley Tree

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Abstract: We study the phase diagram for Potts model on a Cayley tree with competing prolonged ternary and nearest-neighbor interactions. Recently Ganikhodjaev et al.(19) proved that the phase diagram of Potts model with competing nearest-neighbor and prolonged next-nearest-neighbor interactions contains a modulated phase, as found for similar Ising models on periodic lattices. At vanishing temperature, the phase diagram is fully determined for all values of interaction parameters. We show that the set of modulated phases has very simple structure, namely consist of phases with period 4, so called antiphase.

Keywords: Potts model, Phase transition, Cayley tree.

1. INTRODUCTION

Consideration of spin models with multispin interactions has proved to be fruitful in many fields of physics, ranging from the determination of phase diagrams in metallic alloys and exhibition of new types of phase transition, to site percolation. Systems exhibiting spatially modulated structures, commensurate or incommensurate with the underlying lattice, are of current interest in condensed matter physics (1). Among the idealized systems for modulated ordering, the axial next-nearest-neighbor Ising (ANNNI) model, originally introduced by Elliot (2) to describe the sinusoidal magnetic structure of Erbium, and the chiral Potts model, introduced by Ostlund (3) and Huse (4) in connection with monolayers adsorbed on rectangular substrates, have been studied extensively by a variety of techniques. A particularly interesting and powerful method is the study of modulated phases through the measure-preserving map generated by the mean-field equations, as applied by Bak (5) and Jensen and Bak (6) to the ANNNI model. The main drawback of the method lies in the fact that thermodynamic solutions correspond to stationary but unstable orbits. However, when these models are defined on Cayley trees, as in the case of the Ising model with competing interactions examined by Vannimenus (10), it turns out that physically interesting solutions correspond to the attractors of the mapping. This simplifies the numerical work considerably, and detailed study of the whole phase diagram becomes feasible. Apart from the intrinsic interest attached to the study of models on trees, it is possible to argue that the results obtained on trees provide a useful guide to the more involved study of their counterparts on crystal lattices. The ANNNI model, which consists of an Ising model with nearest-neighbour interactions augmented by competing next-nearest-neighbor couplings acting parallel to a single axis direction, is perhaps the simplest nontrivial model displaying a rich phase diagram with a Lifshitz point and many spatially modulated phases. There has been a considerable theoretical effort to obtain the structure of the global phase diagram of the ANNNI model in the $T-p$ space, where T is temperature and $p = -J_p/J_1$ is the ratio between the competing exchange interactions. On the basis of numerical mean-field calculations, Bak and von Boehm (7) suggested the existence of an infinite succession of commensurate phases, the so-called devil's staircase, at low temperatures. This mean-field picture has been supported by low-temperature series expansions performed by Fisher and Selke (8). At the paramagnetic-modulated boundary analytic mean-field calculations show that the critical wave number varies continuously and vanishes at the Lifshitz point. A phase diagram of a model describes a morphology of phases, stability of phases, transitions from one phase to another and corresponding transitions line. A Potts model just as an Ising model on a Cayley tree with competing interactions has recently been studied extensively because of the appearance of nontrivial magnetic orderings (see (10)-(15), (19)-(22) and references therein). The Cayley tree is not a realistic lattice; however , its amazing topology makes the exact calculation of various quantities possible.

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For many problems the solution on a tree is much simpler than on a regular lattice and is equivalent to the standard Bethe-Peierls theory (16). On the Cayley tree one can consider two type of triple neighbors: prolonged and two-level (definitions see below). In the case of the Ising model with competing nearest-neighbor interactions J and prolonged next-nearest-neighbor interactions Jp Vannimenus (10) was able to find new modulated phases, in addition to the expected paramagnetic and ferromagnetic ones. From this result follows that Ising model with competing interactions on a Cayley tree is real interest since it has many similarities with models on periodic lattices. In fact, it has many common features with them, in particular the existence of a modulated phase, and shows no sign of patological behaviour - at least no more than mean-field theories of similar systems (10). Moreover detailed study of its properties was carried out with essentially exact results, using rather simple numerical methods. This suggest that more complicated models should be studied on trees, with the hope to discover new phases or unusual types of behaviour. The important point is that statistical mechanics on trees involve nonlinear recursion equations and are naturally connected to the rich world of dynamical systems, a world presently under intense investigation (10). The model (1) with $Jp = 0$ was considered in (20)-(21) and proved that phase diagram of this model contains ferromagnetic and antiferromagnetic phases.

In this paper we consider the Potts model with competing triple nearest-neighbor interactions. The Potts model (17) was introduced as a generalization of the Ising model to more than two components and encompasses a number of problems in statistical physics (see, e.g. (18)) recently. In (19) the phase diagram of the three states Potts model with nearest-neighbor interactions J and prolonged next-nearest- neighbors interactions Jp was described.

2. THE MAIN RESULTS

2.1 The Model

A Cayley tree Γ^k of order $k \geq 1$ is an infinite tree, i.e., a graph without cycles with exactly $k+1$ edges issuing from each vertex. Let denote the Cayley tree as $\Gamma^k = (V, \Lambda)$, where V is the set of vertices of Γ^k, Λ is the set of edges of Γ^k. Two vertices x and y, $x, y \in V$ are called *nearest-neighbors* if there exists an edge $l \in \Lambda$ connecting them, which is denoted by $l =< x, y >$. The distance $d(x, y), x, y \in V$, on the Cayley tree Γ^k, is the number of edges in the shortest path from x to y. For a fixed $x^0 \in V$ we set

$W_n = \{x \in V | d(x, x^0) = n\}, V_n = \{x \in V | d(x, x^0) \leq n\}$
and L_n denotes the set of edges in V_n. The fixed vertex x^0 is called the 0-th level and the vertices in W_n are called the n-th level. For the sake of simplicity we put $|x| = d(x, x^0)$, $x \in V$. Two vertices $x, y \in V$ are called *the next-nearest-neighbors* if $d(x, y) = 2$. Three vertices x, y and z are called a triple of neighbors and they are denoted by $< x, y, z >$, if $< x, y >, < y, z >$ are nearest neighbors.The triple of vertices x, y, z is called *prolonged* if $x \in W_n, y \in W_{n+1}$ and $z \in W_{n+2}$ for some nonnegative integer n and is denoted by $< \widetilde{x, y, z} >$. The triple of vertices $x, y, z \in V$ that are not prolonged is called *two-level* since $|x| = |z|$ and are denoted by $< x, \bar{y}, z >$.

Below we will consider a semi-infinite Cayley tree Γ^2_+ of second order , i.e. an infinite graph without cycles with 3 edges issuing from each vertex except for x^0 which has only 2 edges.

For the three-state Potts model with spin values in $\Phi = \{1, 2, 3\}$, the relevant Hamiltonian with competing binary nearest-neighbor and ternary interactions has the form

$$H(\sigma) = -J_p \sum_{<\widetilde{x,y,z}>} \delta_{\sigma(x)\sigma(y)\sigma(z)} - J_1 \sum_{<x,y>} \delta_{\sigma(x)\sigma(y)} \quad (1)$$

where $J_p, J_1 \in R$ are coupling constants and δ is the Kronecker symbol. Here the generalized Kronecer's symbol $\delta_{\sigma(x)\sigma(y)\sigma(z)}$ is

$$\delta_{\sigma(x)\sigma(y)\sigma(z)} = \begin{cases} 1 \text{ if } \sigma(x) = \sigma(y) = \sigma(z) \\ 0 \text{ otherwise.} \end{cases}$$

The model (1) with $J_p = 0$ was considered in (12),(13),(20), (21) and proved that phase diagram of this model contains ferromagnetic and antiferromagnetic phases. Below we consider model (1) with $J_p \neq 0$, and and describe its phase diagram.

2.2 Basic Equations

In order to produce the recurrent equations, we consider the relation of the partition function on V_n to the partition function on subsets of V_{n-1}. Given the initial conditions on V_1, the recurrence equations indicate how their influence propagates down the tree. Let $Z^{(n)}(i_1, i_0, i_2)$ be the partition function on V_n where the spin in the root x^0 is i_0 and the two spins in the proceeding ones are i_1 and i_2, respectively. There are 27 different partition functions $Z^{(n)}(i_1, i_0, i_2)$ and the partition function $Z^{(n)}$ in volume V_n can the be written as follows

$$Z^{(n)} = \sum_{i_1, i_0, i_2 = 1}^{3} Z^{(n)}(i_1, i_0, i_2).$$

Next, if it is calculated then we have the following equations

$$\begin{aligned}
Z^{(n)}(1,1,1) &= a^2 Z^{(n)}(1,1) Z^{(n)}(1,1),\\
Z^{(n)}(1,1,2) &= a Z^{(n)}(1,1) Z^{(n)}(1,2),\\
Z^{(n)}(1,1,3) &= a Z^{(n)}(1,1) Z^{(n)}(1,3),\\
Z^{(n)}(2,1,1) &= a Z^{(n)}(1,2) Z^{(n)}(1,1),\\
Z^{(n)}(2,1,2) &= Z^{(n)}(1,2) Z^{(n)}(1,2),\\
Z^{(n)}(2,1,3) &= Z^{(n)}(1,2) Z^{(n)}(1,3),\\
Z^{(n)}(3,1,1) &= a Z^{(n)}(1,3) Z^{(n)}(1,1),\\
Z^{(n)}(3,1,3) &= Z^{(n)}(1,3) Z^{(n)}(1,3),\\
Z^{(n)}(3,1,2) &= Z^{(n)}(1,3) Z^{(n)}(1,2),\\
Z^{(n)}(1,2,1) &= Z^{(n)}(2,1) Z^{(n)}(2,1),\\
Z^{(n)}(1,2,2) &= a Z^{(n)}(2,1) Z^{(n)}(2,2),\\
Z^{(n)}(1,2,3) &= Z^{(n)}(2,1) Z^{(n)}(2,3),\\
Z^{(n)}(2,2,1) &= a Z^{(n)}(2,2) Z^{(n)}(2,1),
\end{aligned}$$

$$
\begin{aligned}
Z^{(n)}(2,2,2) &= a^2 Z^{(n)}(2,2)Z^{(n)}(2,2),\\
Z^{(n)}(2,2,3) &= aZ^{(n)}(2,2)Z^{(n)}(2,3),\\
Z^{(n)}(3,2,1) &= Z^{(n)}(2,3)Z^{(n)}(2,1),\\
Z^{(n)}(3,2,2) &= aZ^{(n)}(2,3)Z^{(n)}(2,2),\\
Z^{(n)}(3,2,3) &= Z^{(n)}(2,3)Z^{(n)}(2,3),\\
Z^{(n)}(1,3,1) &= Z^{(n)}(3,1)Z^{(n)}(3,1),\\
Z^{(n)}(1,3,2) &= Z^{(n)}(3,1)Z^{(n)}(3,2),\\
Z^{(n)}(1,3,3) &= aZ^{(n)}(3,1)Z^{(n)}(3,3),\\
Z^{(n)}(2,3,2) &= Z^{(n)}(3,2)Z^{(n)}(3,2),\\
Z^{(n)}(2,3,1) &= Z^{(n)}(3,2)Z^{(n)}(3,1),\\
Z^{(n)}(2,3,3) &= aZ^{(n)}(3,2)Z^{(n)}(3,3),\\
Z^{(n)}(3,3,1) &= aZ^{(n)}(3,3)Z^{(n)}(3,1),\\
Z^{(n)}(3,3,2) &= aZ^{(n)}(3,3)Z^{(n)}(3,2),\\
Z^{(n)}(3,3,3) &= a^2 Z^{(n)}(3,3)Z^{(n)}(3,3).
\end{aligned}
$$

We can select only six variables $Z^{(n)}(1,1,1)$, $Z^{(n)}(2,1,2)$, $Z^{(n)}(3,1,3)$, $Z^{(n)}(1,2,1)$, $Z^{(n)}(2,2,2)$,$Z^{(n)}(3,3,3)$, and with the introduction of new variables

$$
\begin{aligned}
u_1^{(n)} &= \sqrt{Z^{(n)}(1,1,1)},\ u_2^{(n)} = \sqrt{Z^{(n)}(2,1,2)},\\
u_3^{(n)} &= \sqrt{Z^{(n)}(3,1,3)},\ u_4^{(n)} = \sqrt{Z^{(n)}(1,2,1)},\\
u_5^{(n)} &= \sqrt{Z^{(n)}(2,2,2)},\ u_6^{(n)} = \sqrt{Z^{(n)}(3,3,3)},
\end{aligned}
$$

straightforward calculations show that

$$
\begin{aligned}
u_1^{(n+1)} &= a(bu_1^{(n)} + u_2^{(n)} + u_3^{(n)})^2,\\
u_2^{(n+1)} &= (u_3^{(n)} + u_4^{(n)} + u_5^{(n)})^2,\\
u_3^{(n+1)} &= (u_2^{(n)} + u_4^{(n)} + u_6^{(n)})^2,\\
u_4^{(n+1)} &= (u_1^{(n)} + u_2^{(n)} + u_3^{(n)})^2,\\
u_5^{(n+1)} &= a(u_3^{(n)} + u_4^{(n)} + bu_5^{(n)})^2,\\
u_6^{(n+1)} &= a(u_2^{(n)} + u_4^{(n)} + bu_6^{(n)})^2,
\end{aligned}
\tag{2}
$$

where $a = \exp(\beta J_1); b = \exp(\beta J_p)$.

The total partition function is given in terms of (u_i) by

$$
\begin{aligned}
Z^{(n)} = \quad & (u_1^{(n)} + u_2^{(n)} + u_3^{(n)})^2 + (u_3^{(n)} + u_4^{(n)} + u_5^{(n)})^2\\
&+ (u_2^{(n)} + u_4^{(n)} + u_6^{(n)})^2.
\end{aligned}
\tag{3}
$$

Note that, for boundary condition $\bar{\sigma_n}(V \setminus V_n) \equiv 1$ we have $Z^{(n)}(2,1,2) = Z^{(n)}(3,1,3)$, and $Z^{(n)}(2,2,2) = Z^{(n)}(3,3,3)$, i.e., $u_2 = u_3$ and $u_5 = u_6$.

For discussing the phase diagram, the following choice of reduced variables is convenient:

$$
x = \frac{u_2 + u_4}{u_1 + u_6}, \quad y_1 = \frac{u_1 - u_6}{u_1 + u_6},
$$

$$
y_2 = \frac{u_2 - u_4}{u_1 + u_6}.
$$

The variable x is just a measure of the frustration of the nearest-neighbor bonds and is not an order parameter like y_1, and y_2. Equations (2) yield:

$$
\begin{aligned}
x' &= \frac{1}{aD}(2x + y_2 + 1)^2 + (y_1 + y_2)^2;\\
y_1' &= \frac{1}{D}2(2x + y_2 + b)(by_1 + y_2);\\
y_2' &= -\frac{1}{aD}2(2x + y_2 + 1)(y_1 + y_2);
\end{aligned}
\tag{4}
$$

where

$$
D = (b + 2x)^2 + (by_1 + y_2)^2 + (2b + 4x + y_2)y_2.
$$

The average magnetization m for the nth generation is given by

$$
m = 2 - \frac{4(y_1 + y_2)(2x + y_1 + y_2 + 1)}{(2x + y_1 + 2y_2 + 1)^2 + 2(2x + 1 - y_1)^2}. \tag{5}
$$

Below we use numerical methods to study its detailed behaviour.

2.3 Morphology of the Phase Diagram

It is convenient to know the broad features of the phase diagram before discussing the different transitions in more detail. This can be achieved numerically in a straightforward fashion. The recursion relations (4) provide us the numerically exact phase diagram in $(T/J_1, -J_p/J_1)$ space. Let $T/J_1 = \alpha, -J_p/J_1 = \beta$ and respectively $a = \exp(\alpha^{-1}), b = \exp(-\alpha^{-1}\beta)$. Starting from initial conditions

$$
x^{(1)} = \frac{b^2 + a^2}{(a^3 b^2 + a)}, \quad y_1^{(1)} = \frac{a^2 b - 1}{a^2 b + 1},
$$
$$
y_2^{(1)} = \frac{b^2 - a^2}{(a^3 b^2 + a)},
$$

that corresponds to boundary condition $\bar{\sigma}^{(n)} \equiv 1$, one iterates the recurrence relations (4) and observes their behavior after a large number of iterations. In the simplest situation a fixed point (x^*, y_1^*, y_2^*) is reached. It corresponds to a paramagnetic phase if $y_1^* = 0, y_2^* = 0$ or to a ferromagnetic phase if $y_1^*, y_2^* \neq 0$. Since the form of spins of the Potts model is unessential one can replace the set of spin values $\{1,2,3\}$ by the centered set $\{-1,0,1\}$. Then the average magnetization $\tilde{m}$ for the $n$the generation is given by

$$
\tilde{m} = -\frac{4(y_1 + y_2)(2x + y_1 + y_2 + 1)}{(2x + y_1 + 2y_2 + 1)^2 + 2(2x + 1 - y_1)^2}. \tag{6}
$$

Thus a situation where $y_1^*, y_2^* \neq 0$ but $\tilde{m} = 0$ cannot occur (with respect to centered set of spins).

Secondary, the system may be periodic with period p, where case $p = 2$ corresponds to antiferromagnetic phase and case $p = 4$ corresponds to so-called antiphase, that denoted $< 2 >$ for compactness. Finally, the system may remain aperiodic. The distinction between a truly aperiodic case and one with a very long period is difficult to make numerically. Below we consider periodic phases with period p where $p \leq 12$. All periodic phases with period $p > 12$ and aperiodic phase we will consider as modulated phase. The resultant phase diyagram is shown that in Figure 1.

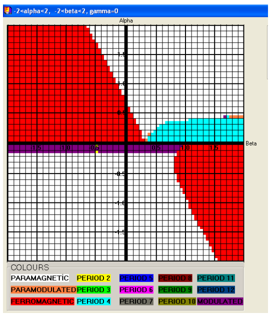

Fig. 1. Phase diagram of Potts model (1)

3. CONCLUSION

In (19) proved that the phase diagram of Potts model with competing nearest-neighbor and prolonged next-nearest-neighbor interactions consists of five phases : ferromagnetic, paramagnetic, modulated, antiphase and paramodulated phases. We have found the phase diagram of the Potts model with competing prolonged ternary and binary nearest-neighbor interactions on the Cayley tree of second order and show that it consists of three phases only: ferromagnetic, paramagnetic and antiphase with period 4. Thus for considered model one can reach periodic phase with period 4 only, i.e., the set of modulated phases has simplest structure.

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