Phase Diagram of the Blume-Emery-Griffiths-Vannimenus Model on the Cayley Tree

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Abstract. We study the phase diagram of the Blume-Emery-Griffiths-Vannimenus model on a Cayley tree with competing nearest-neighbour couplings and next-nearest-neighbour couplings and show that a detailed study of its properties can be carried out with essentially exact results, using rather simple numerical methods. In addition to the expected paramagnetic and ferromagnetic phases, we find modulated phase for Blume-Emery-Griffiths model and hence for Blume-Emery-Griffiths-Vannimenus model also.

1. Introduction
The existence of competing interactions lies at the heart of a variety of original phenomena in magnetic systems, ranging from the spin-glass transitions found in many disordered materials to the modulated phases with an infinite number of commensurate regions, that are observed in certain models with periodic interactions [1]. Vannimenus [1] and Mariz et al [2] examine the local properties of the Ising model on a Cayley tree with nearest-neighbour interactions and competing next-nearest-neighbour interactions. By a process of iteration, Vannimenus found a new modulated phase, in addition to the expected paramagnetic, ferromagnetic and antiferromagnetic phases, which consisted of commensurate (periodic) and incommensurate (aperiodic) regions corresponding to the so-called ”devil’s staircase”, found also in the ANNNI [3] and other competing interaction models [4]. As expanded Ising model, the Blume-Emery-Griffiths (BEG) model, which is characterized by bilinear and biquadratic exchange interactions and crystal-field interaction, has played important role in the development of the theory of tricritical phenomena. The Hamiltonian of the BEG model on the Cayley tree is given by

$$H(\sigma) = -J \sum_{<x,y>} \sigma(x)\sigma(y) - K \sum_{<x,y>} \sigma^2(x)\sigma^2(y) + D \sum_x \sigma^2(x)$$  \hspace{1cm} (1)

where $\sigma(x) \in \{-1, 0, 1\}$ is the spin at site $x$, first and second summation run over all the nearest-neighbour pairs, and last summation runs over all the sites. Here $J, K, D$ describe the bilinear exchange, biquadratic interactions, and crystal-field interaction. This Hamiltonian was originally proposed to explain the phase separation and superfluidity in $^3He - ^4He$ mixtures [5]. The present paper is devoted to the study of a Blume-Emery-Griffiths-Vannimenus model on a Cayley tree with competing nearest-neighbour couplings and next-nearest-neighbour couplings and to show that a detailed study of its properties can be carried out with essentially exact results, using rather simple numerical methods.
2. The Blume-Emery-Griffiths-Vannimenus model

The model considered consists of spins \( \{\sigma(x) \in \{-1, 0, 1\}\} \) on a semi-infinite Cayley tree \( \Gamma^2_\infty = (V, L) \) of second order, i.e., an infinite graph without cycles with 3 edges issuing from each vertex except for \( x^0 \), so-called a root of the tree, which has only 2 edges, where \( V \) is the set of vertices and \( L \) is the set of edges. Two kinds of bonds are present: nearest-neighbours interactions and prolonged next-nearest-neighbour interactions, these being restricted to spin belonging to the same branch of the tree.

The Model: The Hamiltonian of the Blume-Emery-Griffiths-Vannimenus (BEGV) model on the Cayley tree is defined by

\[
H(\sigma) = -J_p \sum_{<x,y>} \sigma(x)\sigma(y) - J_1 \sum_{<x,y>} \sigma(x)\sigma(y) - K \sum_{<x,y>} \sigma^2(x)\sigma^2(y) + D \sum_x \sigma^2(x) \tag{2}
\]

where \( \sigma(x) \in \{-1, 0, 1\} \) is the spin at site \( x \in V \), the first summations runs over all prolonged next-nearest-neighbours, the second and third summation runs over all nearest-neighbours pairs, and last summation runs over all the sites. Here \( J_p, J_1, K, D \) describe the bilinear exchange, biquadratic interactions and crystal-field interaction respectively. The Hamiltonian (2) with \( J_p = 0 \) defines the BEG model [5] and with \( K = D = 0 \) defines Vannimenus model [1].

3. Recurrence equations

In order to produce the recurrence equations, we consider the relation of the partition function of an \( n \) - generation tree \( V_n \) to the partition function of its subsystems containing \( (n - 1) \) generations \( V_{n-1} \).

Let \( <x^0, x> \Rightarrow l \in L \) be an edge of semi-infinite Cayley tree \( \Gamma^2_\infty \) of second order. The infinite subtree \( \Gamma^2_\infty(l) = (V^l, L^l) \) is called a single-trunk Cayley tree, if from vertex \( x^0 \) a single edge \( l \) emanates and from any other vertex \( x \in V^l, x \neq x^0 \) exactly 3 edges emanate. Let \( W_1 = \{x_1, x_2\} \) and \( <x^0, x^1> \Rightarrow l_1, <x^0, x^2> \Rightarrow l_2 \) be two edges emanating from \( x^0 \). It is evident that semi-infinite Cayley tree \( \Gamma^2_\infty(l) \) splits into two components - two single-trunk Cayley trees \( \Gamma^2_\infty(l_i), i = 1, 2 \).

Assume \( Z^{(n)}(i, j) \) be a partition function on \( V^i \) with the configuration \( (i, j) \) on an edge \( l = <x^0, x> \), where \( i, j = -1, 0, 1 \); and \( Z^{(n)}(i_1, i_0, i_2) \) be a partition function on \( V_n \) where the spin in the root \( x^0 \) is \( i_0 \) and the two spins in the proceeding vertices \( x^1, x^2 \) 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 be written as follows

\[
Z^{(n)} = \sum_{i_1, i_0, i_2 = -1}^1 Z^{(n)}(i_1, i_0, i_2). \tag{3}
\]

and

\[
Z^{(n)}(\sigma(x^1), \sigma(x^0), \sigma(x^2)) = Z^{(n)}(\sigma(x^0), \sigma(x^1)) \cdot Z^{(n)}(\sigma(x^0), \sigma(x^2)). \tag{4}
\]

Let

\[
a = \exp\left(\frac{J_p}{k_BT}\right), b = \exp\left(\frac{J_1}{k_BT}\right), c = \exp\left(\frac{K}{k_BT}\right), d = \exp\left(-\frac{D}{2k_BT}\right).
\]

From (4) one can select only nine new independent variables

\[
\begin{align*}
    u_1^{(n)} &= \sqrt{Z^{(n)}(-1, -1, -1)}, & u_2^{(n)} &= \sqrt{Z^{(n)}(-1, 0, -1)}, & u_3^{(n)} &= \sqrt{Z^{(n)}(-1, 1, -1)}, \\
    u_4^{(n)} &= \sqrt{Z^{(n)}(0, -1, 0)}, & u_5^{(n)} &= \sqrt{Z^{(n)}(0, 0, 0)}, & u_6^{(n)} &= \sqrt{Z^{(n)}(0, 1, 0)}, \\
    u_7^{(n)} &= \sqrt{Z^{(n)}(1, -1, 1)}, & u_8^{(n)} &= \sqrt{Z^{(n)}(1, 0, 1)}, & u_9^{(n)} &= \sqrt{Z^{(n)}(1, 1, 1)}.
\end{align*}
\]
We note that, in the paramagnetic phase (high symmetry phase), \( u_1 = u_9, u_2 = u_8, u_3 = u_7 \) and \( u_4 = u_6 \). For discussing the phase diagram, the following choice of reduced variables is convenient:

\[
\begin{align*}
 x_1 &= \frac{u_2 + u_8}{u_1 + u_9}, & x_2 &= \frac{u_3 + u_7}{u_1 + u_9}, & x_3 &= \frac{u_4 + u_6}{u_1 + u_9}, & x_4 &= \frac{2u_5}{u_1 + u_9}, \\
y_1 &= \frac{u_4 - u_6}{u_1 + u_9}, & y_2 &= \frac{u_2 - u_8}{u_1 + u_9}, & y_3 &= \frac{u_5 - u_7}{u_1 + u_9}, & y_4 &= \frac{u_4 - u_5}{u_1 + u_9}.
\end{align*}
\]

It is straightforward to establish the following recursive relations:

\[
\begin{align*}
 x'_1 &= \frac{1 + x_2 + x_3}{bcD} + y_1 y_3 + y_4, & y'_1 &= \frac{2(a + a^{-1} x_2 + x_3)(a y_1 - a^{-1} y_1 + y_4)}{bcD}, \\
 x'_2 &= \frac{a^{-1} + ax_2 + x_3}{bcD} + |a^{-1} y_1 - ay_1 + y_4|, & y'_2 &= \frac{2(1 + x_2 + x_3)(y_1 - y_3 + y_4)}{bcD}, \\
 x'_3 &= \frac{(a + a^{-1}) x_1 + x_3}{bcD} + |a^{-1} y_2|, & y'_3 &= \frac{2(a^{-1} + ax_2 + x_3)(a y_1 - ay_1 + y_4)}{bcD}, \\
 x'_4 &= \frac{2x_1 + x_4}{bcD}, & y'_4 &= \frac{2(a - a^{-1})(a + a^{-1}) x_1 + x_4}{bcD} y_2,
\end{align*}
\]

where

\[ D = (a + a^{-1} x_2 + x_3)^2 + (ay_1 - a^{-1} y_3 + y_4)^2, \]

and primed variables correspond to the \( Z^{(n+1)}(t_1, t_0, t_2) \). The system of eight equations (5) are essentially complicated than the similar basic equations of the Ising model [1], [2].

The total partition function is given in terms of \( (u^{(n)}_i) \) by

\[ Z^{(n)} = (u^{(n)}_1 + u^{(n)}_4 + u^{(n)}_7)^2 + (u^{(n)}_2 + u^{(n)}_5 + u^{(n)}_8)^2 + (u^{(n)}_3 + u^{(n)}_6 + u^{(n)}_9)^2. \]

The average magnetization \( m^{(n)} \) for the \( n \)th generation is given by

\[ m^{(n)} = -\frac{4(1 + x_2 + x_3)(y_1 - y_3 + y_4)}{(2x_1 + x_4)^2 + 2(1 + x_2 + x_3)^2 + (y_1 - y_3 + y_4)^2}. \]

4. Phase Diagram

In this chapter we consider the broad features of the phase diagram. This can be achieved numerically in a straightforward fashion. Starting from random initial conditions (with \( y_1, y_2, y_3, y_4 \neq 0 \)), one iterates the recurrence relations (5) and observes their behaviour after a large number of iterations. In the simplest situation a fixed point \( (x'_1, x'_2, x'_3, x'_4, y'_1, y'_2, y'_3, y'_4) \) is reached. It corresponds to a paramagnetic phase (P) if \( y'_1 = y'_2 = y'_3 = y'_4 = 0 \), or to a ferromagnetic phase (F) if \( y'_1, y'_2, y'_3, y'_4 \neq 0 \). 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 (M). We plot phase diagrams in \((k BT/J_1, D/J_1)\) plane for some fixed values of \( p = -J_p/J_1 \) and \( k = K/J_1 \) with \( J_1 > 0 \) and \( D > 0 \).

The phase diagrams of BEG model, i.e., \( J_p = 0 \), are shown in Fig.1. Here \( p = 0 \) and \( k = \pm 0.5 \). One can see that the phase diagram contains modulated phase, in addition to the expected paramagnetic and ferromagnetic ones. As shown by Vannimenus [1] for the Ising model one can reach modulated phase only in presence of competing next-nearest-neighbours interactions, meanwhile for the BEG model with nearest-neighbour interactions we have modulated phase. If \( K > 0 \) then the phase diagram contains paramagnetic, ferromagnetic and modulated phases and all three phases meet at the multicritical point \( (T/J_1 = 1.6, D/J_1 = 1) \), and if \( K < 0 \) then the phase diagram contains ferromagnetic and modulated phases only.
Fig. 1. Phase diagram of BEG model for (a) $K/J_1 = 0.5$ and (b) $K/J_1 = -0.5$

The phase diagrams of BEGV model with $p = 0.6$ and $k = \pm 0.5$ are shown in Fig. 2
If $K > 0$ then the phase diagram contains antiphase and modulated phases only, and if $K < 0$ the phase diagram contains antiphase, modulated phase and regions with period 5, 6, and 9.

Fig. 2. Phase diagram of BEGV model for (a) $K/J_1 = 0.5, -J_p/J_1 = 0.6$ and (b) $K/J_1 = -0.5, -J_p/J_1 = 0.6$

5. Conclusion
We show that the local magnetization for BEG model with nearest-neighbour interactions on a Cayley tree is mainly chaotic with oscillatory glasslike behavior (see [1], [3], [4]) and for BEGV model the local magnetization is fully chaotic. For BEG model on periodic lattice one can expect similar result. The structure of modulated phase and stability of the phases will be considered in another paper.

5.1. Acknowledgments
This work is supported by the FRGS Grant Phase 2/2010, FRGS 10-022-0141.

6. References
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