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The Blume-Emery-Griffiths Model on Cayley Tree and its Phase Transitions

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Abstract: We consider simple version of the Blume-Emery-Griffiths model on the Cayley tree and investigate the problem of phase transition using the exact recursion equations for the Cayley tree of second order, so that every spin has three nearest neighbours. These equations are studied analytical-ly for D>0 and J>0. It is proved that one can reach phase transition if the reduced crystal-field interaction D/J≤2. It is found the exact value for the critical temperature $T_c = (\ln(2+\sqrt{3}))^{-1} J/k_B$ and described the region R_A of phase transition. On the other hand it is described the phase transition region R_N for considered model using numerical methods, namely, we consider three limiting Gibbs measures with different boundary conditions and if at least two of them are different then we have phase transition. It is compared the phase transition regions R_A and R_A.

Key words: Blume-Emery-Griffiths model . phase transition . crystal-field interaction . Gibbs measure . recurrence equations

INTRODUCTION

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. This model was originally proposed to explain the phase separation and superfluidity in ^{3}He-^{4}He mixtures [1] and has been studied by a variety of techniques, e.g., the generalized Bethe-Peierls approximation [2,3], the effective-field theory [1,2], the exact recursion relations method [4] and so on. A phase diagram of the simple version of the BEG model was studied by de Oliveira and Salinas in [2]. Recently T. Morais and A. Procacci [5] have proved the absence of phase transitions in the BEG model on integer lattice Z^d, d≥2. In this paper using the exact recursion relations method we show the existence of phase transitions in the simple version of the BEG model [2] on the Cayley tree of second order and describe phase transition region.

MODEL

The model considered consists of spins {-1,0,1} on a semi-infinite Cayley tree $\Gamma^2 = (V,L)$ 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 vertices x and y in V are called nearest-neighbors if there exists an edge $l\in L$ connecting them, which is denoted by $l = \langle x; y \rangle$. The distance $d(x; y)$; $x; y \in V$, on the Cayley tree Γ^2, is the number of edges in the shortest path from x to y. For a fixed $x^0\in V$ we set

$$W_n = \{x\in V \mid d(x; x^0) = n\};\ V_n = \{x\in V \mid d(x; x^0) \le n\}$$

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. The Hamiltonian of the Blume-Emery-Griffiths (BEG) model on the Cayley tree is defined by

$$H(s) = -J\sum_{\langle x,y\rangle} s(x)s(y) - K\sum_{\langle x,y\rangle} s^2(x)s^2(y) + D\sum_x s^2(x) \qquad (1)$$

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where $\sigma(x)\in\{-1,0,1\}$ is the spin at site $x\in V$, the first and the second summation runs over all nearest-neighbours pairs and third summation runs over all the sites. Here J,K and D describe the bilinear exchange, biquadratic interactions and crystal-field interaction respectively. Below we will consider simple version of BEG model when K = 0 [2].

RECURRENCE EQUATIONS

There are several approaches to derive equation or system equations describing limiting Gibbs measures for lattice models on Cayley tree [3], [6]. One approach is based on recursive equations for partition functions. Let Λ be a finite subset of V. We will denote by $s(\Lambda)$ the restriction of a configuration s to Λ. Let $\omega(V\setminus\Lambda)$ be a fixed configuration. The total energy of configuration $s(\Lambda)$ under boundary condition $\omega(V\setminus\Lambda)$ is defined as

$$H(\sigma(\Lambda)\,|\,\omega(V\setminus\Lambda)) = -J\sum_{\substack{<x,y>\\ x,y\in\Lambda}}\sigma(x)\sigma(y) - J\sum_{\substack{<x,y>\\ x\in\Lambda,\, y\notin\Lambda}}\sigma(x)\omega(y) + D\sum_{x\in\Lambda}\sigma^2(x) \tag{2}$$

Then partition function in volume Λ under fixed configuration is defined as

$$Z_\Lambda(\omega(V\setminus\Lambda)) = \sum_{\sigma(\Lambda)\in\Omega(\Lambda)}\exp(-\beta H(\sigma(\Lambda)\,|\,\omega(V\setminus\Lambda)) \tag{3}$$

where $\Omega(\Lambda)$ is the set of all configurations in volume Λ and $\beta = 1/k_BT$ is the inverse temperature, where k_B is the Boltzman constant. Then conditional Gibbs measure μ_Λ of a configuration $\sigma(\Lambda)$ is defined as

$$m_\Lambda(s(\Lambda)\,|\,w(V\setminus\Lambda)) = \frac{\exp(-bHs(\Lambda\,|\,w(V\setminus\Lambda))}{Z_\Lambda(w(V\setminus\Lambda))} \tag{4}$$

Let if $\Lambda = V_n$, a configuration, partition function and conditional Gibbs measure in volume V_n denote as σ_n, $Z^{(n)}$ and μ_n respectively. Let $Z_i^{(n)}$ be the partial partition functions with the spin i in the root x^0, i = -1,0,1, i.e.,

$$Z_i^{(n)} = \sum_{\sigma_n\in\Omega_n:\sigma_n(x^0)=i}\exp(-\beta H(\sigma_n\,|\,\omega(V\setminus V_n))$$

with

$$Z^{(n)} = Z_{-1}^{(n)} + Z_0^{(n)} + Z_1^{(n)}$$

In order to produce the recurrent equations we consider the relation of the partition function on V_{n+1} to the partition function on subsets of V_n. Simple algebra gives

$$\begin{aligned} Z_{-1}^{(n+1)} &= c\left[aZ_{-1}^{(n)} + Z_0^{(n)} + a^{-1}Z_1^{(n)}\right]^2 \\ Z_0^{(n+1)} &= \left[Z_{-1}^{(n)} + Z_0^{(n)} + Z_1^{(n)}\right]^2 \\ Z_{-1}^{(n+1)} &= c\left[a^{-1}Z_{-1}^{(n)} + Z_0^{(n)} + aZ_1^{(n)}\right]^2 \end{aligned} \tag{5}$$

where a = exp(ßJ) and c = exp(-ßD). It is evident from (4) that

$$\mu_n\left(\{\sigma_n : \sigma_n(x^0) = i\}\right) = \frac{Z_i^{(n)}}{Z^{(n)}} \tag{6}$$

Let $u_n = Z_{-1}^{(n)} / Z_0^{(n)}$ and $v_n = Z_1^{(n)}/Z_0^{(n)}$. Then from (5) one can produce the following system of recurrent equations

$$u_{n+1} = c\left[\frac{au_n + a^{-1}v_n + 1}{u_n + v_n + 1}\right]^2,\; v_{n+1} = c\left[\frac{a^{-1}u_n + av_n + 1}{u_n + v_n + 1}\right]^2 \tag{7}$$

If $u = \lim_{n\to 8} u_n$ and $v = \lim_{n\to 8} v_n$, then these equations are reduced to following system of nonlinear equations

$$u = c\left[\frac{au + a^{-1}v + 1}{u + v + 1}\right]^2, \; v = c\left[\frac{a^{-1}u + av + 1}{u + v + 1}\right]^2 \tag{8}$$

The solutions of this system (8) describe translation-invariant Gibbs measures (see [6]) and if for some fixed values of parameters a and c the system (8) has more than one solution then phase transition is occurred.

PHASE TRANSITION REGION

In this section we describe solutions of the system of nonlinear equations (8):

$$u = c\left[\frac{au + a^{-1}v + 1}{u + v + 1}\right]^2, \; v = c\left[\frac{a^{-1}u + av + 1}{u + v + 1}\right]^2$$

Subtracting these equations, we have

$$u - v = \frac{(a - a^{-1})c(u - v)[(a + a^{-1})(u + v) + 2]}{[u + v + 1]^2} \tag{9}$$

So that the equality u=v give us some solutions. In this case one of these equations one can rewrite as

$$c^{-1}u = \left[\frac{(a + a^{-1})u + 1}{2u + 1}\right]^2 \tag{10}$$

Let us consider the function

$$f(u) = \left[\frac{(a + a^{-1})u + 1}{2u + 1}\right]^2$$

with

$$f'(u) = \frac{2(a + a^{-1} - 2)[(a + a^{-1})u + 1]}{(2u + 1)^3} \quad \text{and} \quad f''(u) = \frac{2(a + a^{-1} - 2)[(a + a^{-1})u - (a + a^{-1}) + 6]}{(2u + 1)^4}$$

Since $a + a^{-1} > 2$ for any a, the function f(u) is increasing for u > 0 and there exists single inflection point

$$u_{imf} = \frac{(a + a^{-1}) - 6}{4(a + a^{-1})}$$

If $a + a^{-1} < 6$, then $u_{inf} < 0$ and for all u>0 we have $f' > 0$ and $f'' > 0$, i.e., the function f(u) is increasing and convex, such that the equation (10) has a single root.

Lemma 1: Let $a + a^{-1} > 6$. Then there exist $\eta_1(a)$, $\eta_2(a)$ with $0 < \eta_1(a) < \eta_2(a)$ such that the equation (10) has three solutions if

$$\eta_1(a) < c^{-1} < \eta_2(a) \tag{11}$$

has two solutions if either $c^{-1} = \eta_1(a)$ or $c^{-1} = \eta_2(a)$ and has single solution for other cases. In fact,

$$h_i(a) = \frac{1}{u_i^*} f(u_i^*)$$

where u_1^* and u_2^* are the solutions of the equation

$$uf' = f(u) \tag{12}$$

Proof: Let $a + a^{-1} > 6$. Then $u_{inf} > 0$, $f' > 0$ and $f'' > 0$ for $0 < u < u_{inf}$ and $f'' < 0$ for $u > u_{inf}$. The equation (12) is equivalent to

$$2(a + a^{-1})u^2 - (a + a^{-1} - 6)u + 1 = 0 \tag{13}$$

That has two positive roots if $a + a^{-1} > 18$ and single root if $a + a^{-1} = 18$. Using simple calculus one can show that if $a + a^{-1} > 18$ and $\eta_1(a) < c^{-1} < \eta_2(a)$ then the equation (10) has three positive roots

$$\tilde{u}_1 < \tilde{u}_2 < \tilde{u}_3$$

where first and third roots are stable and second one unstable.
Now let us come back to equation (9). After cancelling by (u-v) we have

$$t^2 + [2 - c(a^2 + a^{-2})]t + [1 - 2c(a - a^{-1})] = 0$$

where t = u+v. Using simple calculus one can show this equation has a single positive root if $c > c_1$ does not have positive root if $c < c^*$ and has two positive roots if $c^* < c < c_1$, where

$$c_1 = \frac{1}{2(a - a^{-1})};\ c^* = \frac{4(a + a^{-1} - 2)}{(a^2 - a^{-2})(a + a^{-1})}$$

Below we describe region in the plane (k_BT/J; D/J) where phase transition is occurred. For brevity assume $x = k_BT/J$ and $z = D/J$. Then $a = \exp(1/x)$ and $c = \exp(-(1/x)z)$. In the case u = v the double inequality (11) one can rewrite as follows

$$\ln h_1(a) < \frac{D}{k_BT} < \ln h_2(a) \quad \text{and} \quad \frac{k_BT}{J}\ln h_1(a) < \frac{D}{J} < \frac{k_BT}{J}\ln h_2(a)$$

Then solving the equation (13) we have

$$u_1^* = \frac{\cosh(x^{-1}) - 3 - \sqrt{(\cosh(x^{-1}) - 1)(\cosh(x^{-1}) - 9)}}{4\cosh(x^{-1})}$$

and

$$u_2^* = \frac{\cosh(x^{-1}) - 3 + \sqrt{(\cosh(x^{-1}) - 1)(\cosh(x^{-1}) - 9)}}{4\cosh(x^{-1})}$$

and respectively

$$h_1(x) = \frac{1}{u_1^*}\left[\frac{2\cosh(x^{-1})u_1^* + 1}{2u_1^* + 1}\right]^2 \quad \text{and} \quad \eta_2(x) = \frac{1}{u_2^*}\left[\frac{2\cosh(x^{-1})u_2^* + 1}{2u_2^* + 1}\right]^2$$

and finally

$$F_1(x) = \ln h_1(x); F_2(x) = \ln h_2(x)$$

Note that the functions $F_1(x)$ and $F_2(x)$ are defined on the segment $[-\ln(9+\sqrt{80}))^{-1}, \ln(9+\sqrt{80}))^{-1}]$, where $\ln(9+\sqrt{80}))^{-1} \sim 0.3463$. Then a region bounded by curves $xF_1(x)$ and $xF_2(x)$ is a phase transition region for BEG model when u = v (Fig. 1).

For second case with $u \neq v$, simple but tedious analysis gives that the system of equations (7) has more than one solution if $J > 0$, $a + a^{-1} > 4$ and

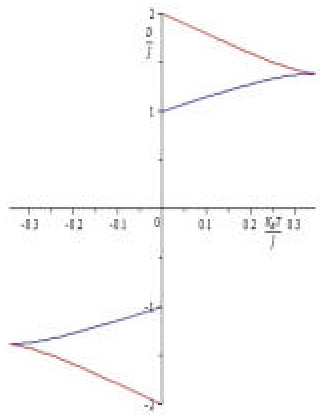

Fig. 1: Phase transition region for BEG model with u = v

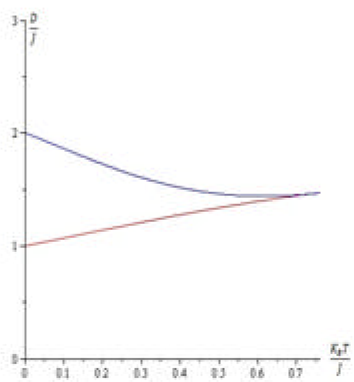

Fig. 2: Phase transition region R_A for simple version of BEG model

$$x\ln 4\sinh(x^{-1}) < z < x\ln\frac{\sinh(x^{-1})\cosh^2(x^{-1})}{\cosh(x^{-1})-1}$$

with $x \in [0, (\ln(2+\sqrt{3}))^{-1}]$. Then a region R_A,defined by these double inequalities, is a phase region for BEG model with K=0 (Fig. 2). One can see that phase transition region in Fig. 2 contains phase transition region in Fig. 1, considered in first quadrant. Thus the phase transition region of BEG model described analytically coincides with region in Fig. 2.

Corollary The critical temperature is equal to $T_c = = (\ln(2+\sqrt{3}))^{-1}J/k_B$ and for $T < T_c$ we can reach phase transition.

NUMERICAL DESCRIPTION OF PHASE TRANSITION REGION

In this section we plot phase transition region for BEG model using numerical method. Let ω^i be a boundary configuration such that $\omega^i(x)=i$ for any $x \in V\backslash V_n$, where i = -1,0,1. For brevity we put $Z^{(n)}(i) = Z^{(n)}(\omega^i)$, i=-1,0,1. Firstly we compute

$$Z_{-1}^{(0)}(i);\ Z_{0}^{(0)}(i);\ Z_{1}^{(0)}(i) \text{ and } Z^{(0)}(i) = Z_{-1}^{(0)}(i) + Z_{0}^{(0)}(i) + Z_{1}^{(0)}(i)$$

for three different boundary configurations

$$\omega^0(x)= -1;\ \omega^0(x)=0 \text{ and } \omega^0(x)=1$$

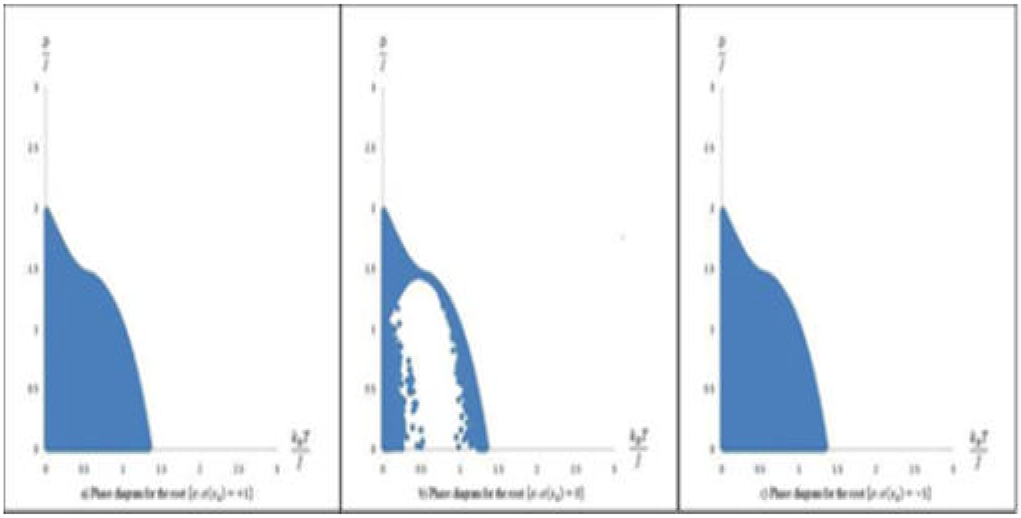

Fig. 3: Phase transition region R_N described by numerical method

respectively. It is evident that

$$Z_{-1}^{(0)}(-1) = ca^{2}; Z_{0}^{(0)}(-1) = 1,; Z_{1}^{(0)}(-1) = ca^{-2}$$

with

$$Z^{(0)}(-1) = ca^{2} + 1 + ca^{-2} \quad \text{and} \quad Z_{-1}^{(0)}(0) = c; Z_{0}^{(0)}(0) = 1,; Z_{1}^{(0)}(0) = c$$

with

$$Z^{(0)}(0) = 2c + 1 \quad \text{and} \quad Z_{-1}^{(0)}(1) = ca^{-2}; Z_{0}^{(0)}(1) = 1,; Z_{1}^{(0)}(1) = ca^{2}$$

with

$$Z^{(0)}(1) = ca^{2} + 1 + ca^{-2}$$

Now using recurrence equations (5) one can compute $Z^{(n)}(i)$ for any n and respectively compute

$$m_n^{(m)}(\{s_n : s_n(x^0) = i\}) = \frac{Z_i^{(n)}(m)}{Z^{(n)}(m)}$$

with i, m = -1,0,1. Let

$$m^{(m)}(\{s : s(x^0) = i\}) = \lim_{n\to\infty} \frac{Z_i^{(n)}(m)}{Z^{(n)}(m)}$$

with i, m = -1,0,1. Then $\mu^{(-1)}$, $\mu^{(0)}$ and $\mu^{(+1)}$ are three limiting Gibbs measures with plus, zero and minus boundary conditions respectively and for each of them we compute measure of the cylinder set $\{\sigma: \sigma(x^0)=i\}$. If for some i at least two of them different then for given a and c we have phase transition. On the plane ($k_BT/J;D/J$) consider a square $0 < k_BT/J = 3$; $0 < D/J = 3$ with network (0.05p;0.05q), where p, q= 1,…,60. If $k_BT/J=0.05p$ and $D/J=0.05q$, then a = exp(1/0.05p) and c = exp(-q/p). If for these parameters a and c we reach phase transition, a point (0.05p;0.05q) is coloured to blue colour, in opposite case - not. The Fig. 3 represents final result for all points point (0.05p;0.05q), where p, q=1,2,..,60.
One can see that for cylinder sets

$$\{\sigma: \sigma(x^0)=1\} \text{ and } \{\sigma: \sigma(x^0)=-1\}$$

the phase transition (blue) regions are the same but for cylinder set $\{\sigma: \sigma(x^0)=0\}$ the phase transition region essentially differ from previous ones. As the final result we can state that the blue region in part a) or c) is the phase transition region described numerically.

CONCLUSION

In this paper we describe phase transition regions R_A and R_N using analytic and numerical methods respectively. One can see that R_A is a subset of R_N since above we could describe part of solutions the equations (8) only. Note that for both cases maximal value of D/J is equal to 2 and this fact allow us to state that from detail analysis of equations (8) we will have $R_A = R_N$, i.e., analytical and numerical methods will give the same result and in this case $T_c = (\ln(2+\sqrt{3}))^{-1} J/k_B$.

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