Pair correlation functions of the Ising type model with spin 1 within two-particle cluster approximation

By

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The Blume-Emery-Griffiths model on hypercubic lattices within the two-particle cluster approximation is investigated. The expressions for the pair correlation functions in \( k \)-space are derived. On the basis of obtained results (at \( k = 0 \)) the static susceptibility of this model on the simple cubic lattice is calculated at various values of the single-ion anisotropy and biquadratic interaction.

1 Introduction

The Blume-Emery-Griffiths (BEG) model

\[
H = - \sum_{i=1}^{N} D_i S_i^2 - \frac{1}{2} \sum_{i,\delta} \left[ K S_i S_{i+\delta} + K' S_i^2 S_{i+\delta} \right] \tag{1}
\]

(where \( S_i = 0, \pm 1 \); \( D_i \) is a single-ion anisotropy energy; \( K \) and \( K' \) are the constants of bilinear and biquadratic short-range interaction; the summation \( i, \delta \) is going over nearest neighbor pairs) was originally proposed for the description of the phase transition (PT) in \( \text{He}^3 - \text{He}^4 \) fluid [1]. This model has been extensively studied not only because of the relative simplicity with which approximate calculations for the model can be carried out and tested.

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as well as of the fundamental theoretical interest arising from the richness of
the phase diagram that is exhibited due to competition of interactions, but
also because versions and extensions of the model can be applied for the de-
scription of simple and multi-component fluids [2–4], dipolar and quadrupolar
orderings in magnets [4–6], crystals with ferromagnetic impurities [4], order-
ing in semiconducting alloys [7], etc. The model has been studied within
mean-field approximation (MFA) [1–5], two-particle cluster approximation
(TPCA) [8–11], effective field theory [12–15], high-temperature series expan-
sions [16], position–space renormalization group calculations [17], and Monte
Carlo simulations [18–21].

For compounds described by pseudospin models with essential short-range
correlations, the cluster approximation (CA) [10, 11, 22–24] is the most nat-
ural many-particle generalization of the MFA. CA not only essentially im-
proves the MFA results for the Ising type model, but also is correct at those
values of the parameters, at which MFA gives qualitatively incorrect results.
Thus CA, in contrast to MFA, does not predict PT for the 1D Ising model
(with only bilinear short-range interaction) with an arbitrary value of spin [9],
correctly responds to the competition between antiferromagnetic biquadratic
interaction and ferromagnetic bilinear interaction in BEG model [10]. Within
CA, an infinite lattice is replaced with a cluster with a fixed number of pseu-
dospins; the influence of rejected sites is taken into account as a single field
ϕ(S), acting on boundary sites of a cluster.

The BEG model has a complicated phase diagram [20, 25]. In [25] the
model was investigated within the constant-coupling approximation (giving
the same results as TPCA) at \( d = \frac{D}{K} < 0 \), \( k' = \frac{K'}{K} > 0 \) for a cubic lattice.
The phase diagram \( (\frac{D}{K'}, \frac{K}{K'}, T) \) and its projection onto the \( (\frac{D}{K'}, \frac{K}{K'}) \) plane were
constructed. The phase transitions were classified. The authors presented
the temperature dependences of dipolar \( m = \langle S \rangle \) and quadrupolar \( q = \langle S^2 \rangle \)
moments for the some interesting sets of parameters. In [20] the BEG model
on a simple cubic lattice was studied within Bethe approximation (giving
the same results as TPCA) and on the basis of the Monte Carlo simulation.
It was shown that for \( d_a < d < -6k' - 6 \) at \( k' < -1 \) (\( d_a \) depends on
\( k' \): \( d_a = 0, -0.6, -1.2 \) for \( k' = -1, -2.25, -3.85 \), respectively) the phase
with two sublattices \( m_A, m_B, q_A, q_B \) exists. The authors were particularly
interested in the such sets of model parameters where different kinds of re-
entrant and double re-entrant phase transitions took place.

The aim of the present paper is to calculate within TPCA the pair corre-
lation functions \( \langle (S_i)^l (S_j)^n \rangle^c = \langle (S_i)^l (S_j)^n \rangle - \langle (S_i)^l \rangle \cdot \langle (S_j)^n \rangle \) (\( l \) and \( n = 1, 2 \))
of the BEG model in \( \mathbf{k} \)-space and to investigate, using the obtained results
(at \( \mathbf{k} = 0 \)) the temperature dependences of static susceptibility of the model
on a simple cubic lattice at various values of the single-ion anisotropy and
biquadratic interaction (in one-sublattice regions of the phase diagram, only).

2 The two-particle cluster approximation

The expression for a free energy within TPCA is constructed on the basis of
one-particle Hamiltonian \( H_1 \)

\[
H_1 = -\tilde{\alpha}_1 S_1 - \tilde{\alpha}_1' S_1^2; \quad \tilde{\alpha}_1 = \Gamma_1 + \sum_{r \in \pi_1} r \varphi_1; \quad \tilde{\alpha}_1' = D_1 + \sum_{r \in \pi_1} r \varphi_1' \quad (2)
\]

(where the site \( r \) is a nearest neighbour of the site 1 \( (r \in \pi_1) \)) and two-particle
Hamiltonian \( H_{12} \)

\[
H_{12} = -2\tilde{\alpha}_1 S_1 - \tilde{\alpha}_2 S_2 - 2\tilde{\alpha}_1' S_1^2 - 1\tilde{\alpha}_2' S_2^2 - KS_1 S_2 - K' S_1^2 S_2^2; \quad (3)
\]
\[1 \tilde{\alpha}_2 = \Gamma_2 + \sum_{r \in \mathcal{R}_2; r \neq 1} r \varphi_2; \quad 1 \tilde{\alpha}_2' = D_2 + \sum_{r \in \mathcal{R}_2; r \neq 1} r \varphi_2' \]

in a usual way [10, 11] (magnetic field \(\Gamma_i \to 0\) is introduced for convenience; \(K > 0\)).

\[
F = -k_B T \left[ (1 - z) \sum_{i} \ln (S \text{e}^{-\beta H_i}) + \frac{1}{2} \sum_{i,k} \ln (S \text{e}^{-\beta H_{ik}}) \right]
\]

(4)

Here \(z\) is the number of nearest neighbours and \(\beta = 1/(k_B T)\). In the case when the fields are uniform, the free energy can be written as:

\[
F = -k_B TN \left[ (1 - z) \ln Z_1 + \frac{z}{2} \ln Z_{12} \right];
\]

(5)

\[
Z_1 = 2e^{\beta \tilde{\alpha}'} \cdot \cosh(\beta \tilde{\alpha}) + 1;
\]

(6)

\[
Z_{12} = 2e^{\beta(2\tilde{\alpha}'+K')} \left( e^{\beta K} \cdot \cosh(2\beta \tilde{\alpha}) + e^{-\beta K} \right) + 4e^{\beta \tilde{\alpha}'} \cdot \cosh(\beta \tilde{\alpha}) + 1,
\]

where

\[
\tilde{\alpha} = \Gamma + z\varphi; \quad \tilde{\alpha}' = D + z\varphi'; \quad \tilde{\alpha} = \Gamma + (z - 1)\varphi; \quad \tilde{\alpha}' = D + (z - 1)\varphi'.
\]

The cluster parameters \(\varphi\) and \(\varphi'\) are found by minimizing the free energy with respect to them. The following system of equation for \(\varphi\) and \(\varphi'\) is obtained:

\[
\frac{e^{\beta \tilde{\alpha}'} \cdot \sinh(\beta \tilde{\alpha})}{Z_1} = \frac{e^{\beta(2\tilde{\alpha}'+K'+K)} \cdot \sinh(2\beta \tilde{\alpha}) + e^{\beta \tilde{\alpha}'} \cdot \sinh(\beta \tilde{\alpha})}{Z_{12}};
\]

(7)

\[
\frac{e^{\beta \tilde{\alpha}} \cdot \cosh(\beta \tilde{\alpha})}{Z_1} = \frac{e^{\beta(2\tilde{\alpha}'+K')} \left[ e^{\beta K} \cdot \cosh(2\beta \tilde{\alpha}) + e^{-\beta K} \right] + e^{\beta \tilde{\alpha}'} \cdot \cosh(\beta \tilde{\alpha})}{Z_{12}}.
\]

Using (7) we can write simple expressions for magnetization \(m = \langle S \rangle\) and quadrupolar moment \(q = \langle S^2 \rangle\):

\[
m = \frac{2e^{\beta \tilde{\alpha}} \cdot \sinh(\beta \tilde{\alpha})}{Z_1}; \quad q = \frac{2e^{\beta \tilde{\alpha}} \cdot \cosh(\beta \tilde{\alpha})}{Z_1}.
\]

(8)
The correlation functions can be found by differentiating the free energy (4) of the system in nonuniform external fields \((\Gamma_i, D_i)\) with respect to these fields. In the case of a \(\Delta\)-dimensional hypercubic lattice the matrix of pair correlation functions (in the uniform fields case) in \(k\)-space has the form [10, 11]:

\[
\left( \begin{array}{cc}
\langle S_k S_{-k} \rangle^c & \langle S_k S_{-k}^2 \rangle^c \\
\langle S_k^2 S_{-k} \rangle^c & \langle S_k^2 S_{-k}^2 \rangle^c
\end{array} \right) = \left( (1 - z)(\hat{G}_1)^{-1} + z(\hat{G}_1 + \hat{G}_{12})^{-1} \right)
+ 4\left[ \hat{G}_1 (\hat{G}_{12})^{-1} \hat{G}_1 - \hat{G}_{12} \right]^{-1} \sum_{a=1}^{\Delta} \sin^2\left(\frac{k_a}{2}\right)^{-1}
\] (9)

(let us note that \(\langle S_k S_{-k}^2 \rangle^c = \langle S_k^2 S_{-k} \rangle^c\)). Here the following matrices of one-particle and two-particle intracluster correlation functions are introduced:

\[
\hat{G}_1 = \left( \begin{array}{cc}
\langle S_1 S_1 \rangle^c_{H_1} & \langle S_1 S_1^2 \rangle^c_{H_1} \\
\langle S_1^2 S_1 \rangle^c_{H_1} & \langle S_1^2 S_1^2 \rangle^c_{H_1}
\end{array} \right), \quad \hat{G}_{12} = \left( \begin{array}{cc}
\langle S_1 S_2 \rangle^c_{H_{12}} & \langle S_1 S_2^2 \rangle^c_{H_{12}} \\
\langle S_1^2 S_2 \rangle^c_{H_{12}} & \langle S_1^2 S_2^2 \rangle^c_{H_{12}}
\end{array} \right). \quad (10)
\]

3 Numerical analysis results

In this section we discuss the results of numerical calculations within TPCA for temperature dependences of static susceptibility \(\chi = \beta \langle S_k S_{-k} \rangle^c|_{k=0}\) of BEG model on a simple cubic lattice \((z = 6)\).

Here we use the following notations for the relative quantities: \(t = (3k_B T)/(2zK)\), \(d = D/K\), \(k' = K'/K\); and the terminology of [25]: \(\mathbf{F}\) – the ferromagnetic phase \((m \neq 0, q \neq \frac{2}{3})\), \(\mathbf{P}\) – the paramagnetic phase \((m = 0, q \neq \frac{2}{3}, q(t \rightarrow \infty) = \frac{2}{3})\), \(\mathbf{Q}\) – the quadrupolar phase \((m = 0, q \neq \frac{2}{3})\). In the two-particle cluster approximation the system of equations for \(\varphi, \varphi'\ (7)\) has several solutions, the number of which depends on values of parameters \(d, k'\) and temperature. Solution corresponding to the \(\mathbf{P}\) phase exists at \(t \in [t_{P_1}, \infty]\)
\( t_{p_1} \geq 0 \), its value depends on \( d, k' \). Solutions corresponding to the \( \mathbf{F} \) phase and \( \mathbf{Q} \) phase exist at \( t \in [t_{F_1}, t_{F_2}] \) and \( t \in [t_{Q_1}, t_{Q_2}] \), respectively. The values of \( t_{F_1}, t_{F_2} \) and \( t_{Q_1}, t_{Q_2} \) depend on \( d, k' \) and are finite.

The projection of the phase diagram on \((d, k')\) plane for ferromagnetic bilinear interaction at \( d < 0, k' > 0 \) [25] and \( d \geq 0, k' > -1 - \frac{1}{6}d \) (see fig. 1) consists of seven regions: I – the first order phase transition \( \mathbf{Q} \leftrightarrow \mathbf{P} \) (\( \mathbf{QP} \)), II – the PT \( \mathbf{FP}_2 \), III – the PT \( \mathbf{FP}_1 \), IV – the PT is absent (the system is in the \( \mathbf{P} \) phase), V – the PTs \( \mathbf{QF}_1 \) and \( \mathbf{FP}_2 \), VI – the PTs \( \mathbf{QF}_1 \) and \( \mathbf{FP}_1 \), VII – the PTs \( \mathbf{FQ}_1 \) and \( \mathbf{QP}_1 \).

Let us consider now the temperature dependence of the inverse static susceptibility \( \chi^{-1}(t) \) along with quadrupolar moment \( q(t) \) (the latter has been already studied in Ref. [25]). In the \( \mathbf{F} \) phase \( q(t) \) and \( \chi^{-1}(t) \) decrease as \( t \) increases (see figs. 2-6). In the \( \mathbf{Q} \) phase \( q(t) \) increases and \( \chi^{-1}(t) \) decreases (see figs. 5-7). In the \( \mathbf{P} \) phase the situation is more complicated. Depending on the model parameters, \( q(t) \) can decrease or increase, and \( \chi^{-1}(t) \) can be an increasing function (see figs. 2, 6, 7) or a non-monotonic function with one minimum (see figs. 3-5). At infinitely high temperature \( \chi(t \rightarrow \infty) = 2/3 \cdot \beta \).

It should be noted that at any ferromagnetic set of the model parameters \((d \geq 0, k' \geq 0)\), the quadrupolar moment (in the \( \mathbf{P} \) phase) is lowered down by \( t \), and at \((d, k')\) from region IV it is raised up. The fact that decreasing behavior of \( q(t) \) in the \( \mathbf{P} \) phase is changed to an increasing one is caused by decreasing of \( d \) or \( k' \). At the set of the model parameters from regions II or V, \( \chi^{-1}(t) \) in the \( \mathbf{P} \) phase is an increasing function, and at \((d, k')\) from region IV it is a non-monotonic function. Non-monotonic behavior of \( \chi^{-1}(t) \) in the \( \mathbf{P} \) phase is possible only at those \( d \) and \( k' \), at which \( q(t) \) increases in the \( \mathbf{P} \) phase. That is, for instance, increasing of antiferromagnetic \( d \) at constant...
ferromagnetic $k'$ must give rise, first, to increasing of $q(t)$, and only then to non-monotonic behavior of $\chi^{-1}(t)$.

At those sets of the model parameters when the phase transition \textbf{FP2} takes place in the system as $t$ increases (region II and V; see fig. 6) $q(t_c)$ and $\chi^{-1}(t_c)$ have cusps ($\chi^{-1}(t_c) = 0$) at the transition point. In the \textbf{P} phase, as has been already mentioned, $\chi^{-1}(t)$ can only increase, and $q(t)$ can either decrease or increase. Increasing of $q(t)$ is possible only in a small part of region II at $-3 < k' < 1.5$ and sufficiently small $d$ (near the regions III or $d \geq 0$, $k' < -1 - \frac{1}{6}d$).

At those sets of the model parameters when the phase transition \textbf{FP1} takes place in the system (regions III and VI; see figs. 2-4) $q(t_c)$ and $\chi^{-1}(t_c)$ have finite jumps at the transition point, and only $q(t_c)$ always has a downward one ($q(t_c - 0) > q(t_c + 0)$). All possible combinations of the $\chi^{-1}(t_c)$ jump and behaviors of $\chi^{-1}(t)$ and $q(t)$ in the \textbf{P} phase, depending on the model parameters, are the following:

|         | 1 | 2 | 3 | 4 |
|---------|---|---|---|---|
| $q(t)$  | ↘ | ↗ | ↗ | ↗ |
| $\chi^{-1}(t)$ | ↗ | ↗ | ↘ | ↘ |
| $\chi^{-1}(t_c)$ | ↓ | ↓ | ↓ | ↑ |

(hereafter we use the following notations: ↗(↘) – increasing (decreasing) function, ↘↗ – non-monotonic function with one minimum, ↑(↓) – function has a finite upward (downward) jump). The combinations 1,3,4 are presented in figs. 2-4, respectively. It should be noted that an upward jump of $\chi^{-1}(t_c)$ (which can take place only in a small part of region III) is possible when $\chi^{-1}(t)$ is non-monotonic function in the \textbf{P} phase, only. Thus,
increasing of antiferromagnetic $d$ (or decreasing of ferromagnetic $k'$), first
must induce a non-monotonic behavior of $\chi^{-1}(t)$, and only then an upward
jump of $\chi^{-1}(t_c)$. But it is possible (depending on $k'$) that further increas-
ing of antiferromagnetic $d$ leads to a downward jump of $\chi^{-1}(t_c)$ again. For
instance, the sequences of presented combinations of $\chi^{-1}(t_c)$ jump and be-
haviors of $q(t)$ and $\chi^{-1}(t)$ in the $P$ phase as antiferromagnetic $d$ increases (at
given $k'$) are: 2, 3 at $k' = 0.0$; 1, 2, 3, 4, 3 at $k' = 2.0$; 1, 2, 3, 4 at $k' = 2.6$;
1, 2 at $k' = 2.95$; at $k' = 3.2$ the combination 1 is possible only (at $k' = 0.0$
$q(t)$ becomes increasing yet in the region II). It should also be noted that an
upward jump of $\chi^{-1}(t_c)$ and concavity of the $q(t)$ curve in the $P$ phase at
low temperatures (as in fig. 4), are independent phenomena.

At those sets of the model parameters, when the phase transition QP1
takes place in the system (regions I and VII; see figs. 5, 7) at the transition
point $q(t_c)$ and $\chi^{-1}(t_c)$ have finite upward and downward jumps, respectively.
In the $P$ phase, behaviors of $q(t)$ and $\chi^{-1}(t)$ can be the following:

|   | 1 | 2 | 3 |
|---|---|---|---|
| $q(t)$ | $\downarrow$ | $\uparrow$ | $\uparrow$ |
| $\chi^{-1}(t)$ | $\uparrow$ | $\uparrow$ | $\downarrow$ |

(the first and third combinations are presented in figs. 7 and 5, respectively). It should be remembered that the order of presented combinations of
quadrupolar moment and inverse static susceptibility temperature behaviors
in the $P$ phase corresponds to increasing of antiferromagnetic $d$ (or decreasing
of ferromagnetic $k'$). For instance, as antiferromagnetic $d$ increases, the
sequence of presented combinations is 2, 3 at $k' = 2.95$ and 1, 2, 3 at $k' = 4.0$
(at $k' = 2.95$ $q(t)$ becomes increasing yet in the region III).
At the FQ1 phase transition (region VII; see fig. 5) \( q(t_c) \) and \( \chi^{-1}(t_c) \) have finite downward and upward jumps, respectively. At the QF1 transition (regions V, VI; see fig. 6) the situation is reverse \( q(t_c) \) has an upward jump, and \( \chi^{-1}(t_c) \) has a downward one).

Let us note that the projection of the phase diagram on \((d, k'}) plane at \(d < 0, k' < 0\) and \(d \geq 0, k' < -1 - \frac{1}{6}d\) is also complicated [20], and study of static susceptibility at those sets of model parameters is subject of a separate paper.

### 4 Conclusions

In the present paper, the pair correlation functions in \(k\)-space for the Blume-Emery-Griffiths model have been obtained.

The temperature dependences of static susceptibility at various values of model parameters have been investigated. It was shown that in the paramagnetic phase it can be a non-monotonic function of temperature with one maximum. Such behavior is impossible at those sets of the model parameters, when the second order phase transition ferromagnet – paramagnet takes place, and becomes possible after the first order phase transitions from the ferromagnetic or quadrupolar phases (only when the quadrupolar moment in the paramagnetic phase is an increasing function).

It should be noted that if we know the temperature dependences of quadrupolar moment and static susceptibility only in a narrow temperature interval, and those quantities increase (furthermore, the curve of quadrupolar moment temperature dependence is concave), that does not suffice to state that the system is in a quadrupolar, not in a paramagnetic phase. However,
either decreasing of static susceptibility, or convexity (concavity) of the increasing (decreasing) quadrupolar moment curve is enough to state that the system is in the paramagnetic, not in the quadrupolar phase.
Figure 1: The projection of the phase diagram onto $(d,k')$ plane.
Figure 2: The temperature dependences of $m$, $q$ and inverse static susceptibility $\chi^{-1}$ at $k' = 2.6$, $d = -10.4$.

Figure 3: The temperature dependences of $m$, $q$ and inverse static susceptibility $\chi^{-1}$ at $k' = 2.6$, $d = -10.63$. 
Figure 4: The temperature dependences of $m$, $q$ and inverse static susceptibility $\chi^{-1}$ at $k' = 2.6$, $d = -10.79$.

Figure 5: The temperature dependences of $m$, $q$ and inverse static susceptibility $\chi^{-1}$ at $k' = 2.88$, $d = -11.61$. 
Figure 6: The temperature dependences of $m$, $q$ and inverse static susceptibility $\chi^{-1}$ at $k' = 3.44$, $d = -13.34$.

Figure 7: The temperature dependences of $q$ and inverse static susceptibility $\chi^{-1}$ at $k' = 4.0$, $d = -15.4$. 
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