TWO-PARTICLE CLUSTER APPROXIMATION FOR ISING TYPE MODEL WITH ARBITRARY VALUE OF SPIN. CORRELATION FUNCTIONS OF BLUME-EMERY-GRIFFITHS MODEL

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The Ising type model with arbitrary value of spin is investigated within the two-particle cluster approximation. For this model on hypercubic lattices the expressions for the pair correlation functions in $\vec{q}$ -space are obtained. For Blume-Emery-Griffiths model ($S = 1$) on a simple cubic lattice with bilinear K , biquadratic K' interactions and single-ion anisotropy D , a projection of the phase diagram on $D/K - K'/K$ plane is constructed. The temperature dependences of $\langle S^z \rangle$, $\langle (S^z)^2 \rangle$ and pair correlation functions at $\vec{q} = 0$ are calculated at various values of parameters D/K and K'/K .

1. Introduction

Among pseudospin systems studied theoretically, a great attention is paid to Ising-type models, that is, to systems with the Hamiltonian containing only z -component of pseudospin. That is so due to relative simplicity with which approximate calculations for these models can be carried out and tested and possibility of their application to a wide class of real objects. Thus, the Blume-Emery-Griffiths model (BEG) corresponding to the Ising-type model with $\eta = 2$ (hereafter $S^z = -\eta, -\eta+2, \dots, \eta-2, \eta$) was proposed for the investigation of phase transitions (PT) in $He_3 - He_4$ mixture [1]. A general form of the Ising-type model with $\eta = 2$ contains extra terms, as compared to the BEG model, like $S_i^z(S_j^z)^2$. It is used [2,3] for description of external pressure influence on ferromagnetics ($\eta = 1$), for investigation of crystals with ferromagnetic ($\eta = 1$) impurities, three-component non-magnetic alloys, two-component lattice liquids etc. The Ising-type model is proved to be useful in studies of tricritical behaviour of anisotropic ferromagnetics $FeCl_2$ and DAG , of pressure-induced structural phase transitions in NH_4Cl and KH_2PO_4 [2,4].

For compounds described by pseudospin models with essential short-range correlations, the cluster expansion method (CEM) [5-7] is the most natural many-particle generalization of the molecular field approximation (MFA). It should be mentioned that the CEM gives much better results at temperatures far from transition point. Within CEM, an infinite lattice is replaced with a cluster with a fixed number of pseudospins, the influence

of rejected sites is taken into account as a single external field $\varphi(S)$, acting on boundary sites of a cluster. The first consistent formulation of the CEM which allows to determine corrections to free energy related to cluster interaction, was made in [8]. The first order of CEM is called cluster approximation.

Despite a number of papers where CEM is applied to calculation of physical characteristics of various substances, we are aware only of a few ones where pseudospin models with a spin value $\eta > 1$ are considered. Thus, in [9] two-particle cluster approximation (TPCA) was applied to Heisenberg model with spin $\eta > 1$, with the dependence of the variational field φ on spin value being neglected. This neglecting gave qualitatively wrong results even for Ising-type model with $\eta = 2$ [3]. In [10] the BEG model was studied within TPCA. Even though the dependence $\varphi(S)$ was taken into account here, the coefficients of expansion of variational fields φ in powers of pseudospin ($\varphi(S) = \varphi^{(1)} + \varphi^{(2)}S$) were taken to be equal, up to constant terms, to $\langle S \rangle$, $\langle S^2 \rangle$, what gave results close to those of MFA.

For investigation of thermodynamic properties of BEG model, other approximate methods also were widely used. In particular, in a series of papers [11-15], equation chains obtained on the basis of Callen identities are closed with the help of the simplest decoupling $\langle S_1 S_2 \dots S_k \rangle \approx \langle S_1 \rangle \langle S_2 \rangle \dots \langle S_k \rangle$. Calculated in such an approximation transition temperature T_c for the case of $\eta = 1$ [16] differs from results of numerical methods more significantly than the T_c calculated in TPCA does.

The PT of the BEG model at negative values of single-ion anisotropy and positive values of bilinear and biquadratic interaction were studied in [17] within the constant-coupling approximation, which results correspond to the TPCA results. The three-dimensional phase diagram was constructed, and temperature dependences of dipole and quadrupolar moments were obtained for some values of Hamiltonian parameters. In [18] the Bethe approximation (results of this approximation also correspond to the TPCA results) was used for investigation of the BEG model at arbitrary values of single-ion anisotropy and biquadratic interaction. Particular attention was paid the case of antiferro biquadratic interaction. Obtained results were compared with those of Monte Carlo method. We also should mention the results of studies of BEG model within the high-temperature expansion [19] and Monte Carlo methods [20,21]. To our best knowledge, only thermodynamic properties of the considered models have been studied so far.

The goal of this work is to develop a two-particle cluster approximation for calculation of thermodynamic characteristics and correlations functions (CF) of Ising-type model with an arbitrary value of spin and investigate the Blume-Emery-Griffiths model within this approximation.

2. Problem formulation

We consider a pseudospin system with $S = S^z = (-\eta, -\eta + 2, \dots, \eta - 2, \eta)$, described by the Hamiltonian

$$\mathcal{H}(\{h^{(\cdot)}\}) = -\beta H = \sum_{n=1}^{\eta} \sum_{i=1}^N h_i^{(n)} S_i^n + \frac{1}{2} \sum_{n=1}^{\eta} \sum_{m=1}^{\eta} \left[\sum_{i,\delta} K^{(nm)} S_i^n S_{i+\delta}^m + \sum_{i,j} J_{ij}^{(nm)} S_i^n S_j^m \right]. \quad (2.1)$$

Here $K^{(nm)}$ and $J_{ij}^{(nm)}$ are the constants of short-range and long-range interactions, respectively; the notation $\mathcal{H}(\{h^{(\cdot)}\})$ means that $\mathcal{H}$ is a function of $(h_1^{(1)}, \dots, h_N^{(1)}, \dots, h_1^{(\eta)}, \dots, h_N^{(\eta)})$. The factor $\beta = (k_B T)^{-1}$ occurring in $h_i^{(n)}$, $K^{(nm)}$, $J_{ij}^{(nm)}$ will be written explicitly only in some final formulas. As a particular case we consider Blume-Emery-Griffiths model ($\eta = 2$) with long-range interaction:

$$\mathcal{H} = \sum_{i=1}^N [\Gamma_i S_i + D_i S_i^2] + \frac{1}{2} \sum_{i,\delta} [K S_i S_{i+\delta} + K' S_i^2 S_{i+\delta}^2] + \frac{1}{2} \sum_{i,j} [J_{ij} S_i S_j + J'_{ij} S_i^2 S_j^2]. \quad (2.2)$$

Here Γ_i is an external field, D_i is a single-ion anisotropy, K and K' are the constants of bilinear and biquadratic short-range interactions; J_{ij} and J'_{ij} are those of long-range interactions.

Within the molecular field approximation in the long-range interaction, the Hamiltonian (2.1) can be expressed as

$$\mathcal{H}(\{h^{(\cdot)}\}) = {}^k \mathcal{H}(\{\mathfrak{a}^{(\cdot)}\}) - \frac{1}{2} \sum_{n=1}^{\eta} \sum_{m=1}^{\eta} \sum_{i,j} J_{ij}^{(nm)} \langle S_i^n \rangle \langle S_j^m \rangle. \quad (2.3)$$

The following notation for the reference Hamiltonian is used

$${}^k \mathcal{H}(\{\mathfrak{a}^{(\cdot)}\}) = \sum_{n=1}^{\eta} \sum_{i=1}^N \mathfrak{a}_i^{(n)} S_i^n + \frac{1}{2} \sum_{n=1}^{\eta} \sum_{m=1}^{\eta} \sum_{i,\delta} K^{(nm)} S_i^n S_{i+\delta}^m, \quad (2.4)$$

$$\mathfrak{a}_i^{(n)} = h_i^{(n)} + \sum_{m=1}^{\eta} \sum_{j=1}^N J_{ij}^{(nm)} \langle S_j^m \rangle. \quad (2.5)$$

The function $\mathcal{F}(\{h^{(\cdot)}\})$ (logarithm of the partition function) within the MFA in the long-range interaction reads:

$$\mathcal{F}(\{h^{(\cdot)}\}) = \ln \text{Sp}_{\{S\}} e^{\mathcal{H}} = {}^k \mathcal{F}(\{\mathfrak{a}^{(\cdot)}\}) - \frac{1}{2} \sum_{n=1}^{\eta} \sum_{m=1}^{\eta} \sum_{i,j} J_{ij}^{(nm)} \langle S_i^n \rangle \langle S_j^m \rangle, \quad (2.6)$$

where ${}^k \mathcal{F}(\{\mathfrak{a}^{(\cdot)}\})$ is a logarithm of the partition function of the reference system (2.4).

Correlation functions (cumulant averages of spin operators calculated with the Gibbs' distribution with $\mathcal{H}$) of the considered model will be evaluated as:

$$\langle (S_{i_1}^{n_1})^{\nu_1} \dots (S_{i_k}^{n_k})^{\nu_k} \rangle^c = \frac{\delta^{\nu_1}}{\delta(h_{i_1}^{(n_1)})^{\nu_1}} \dots \frac{\delta^{\nu_k}}{\delta(h_{i_k}^{(n_k)})^{\nu_k}} \mathcal{F}(\{h^{(\cdot)}\}); \quad (2.7)$$

and CFs of the reference system as:

$${}^k \langle (S_{i_1}^{n_1})^{\nu_1} \dots (S_{i_k}^{n_k})^{\nu_k} \rangle^c = \frac{\delta^{\nu_1}}{\delta(\mathfrak{a}_{i_1}^{(n_1)})^{\nu_1}} \dots \frac{\delta^{\nu_k}}{\delta(\mathfrak{a}_{i_k}^{(n_k)})^{\nu_k}} {}^k \mathcal{F}(\{\mathfrak{a}^{(\cdot)}\}). \quad (2.8)$$

From the expression for the $\mathcal{F}$ -function (2.6) we can easily derive some relations between single-site CFs of the reference system (2.4) and those of the general system within the MFA in long-range interactions (2.3):

$$\langle S_i^n \rangle = \frac{\delta}{\delta(h_i^{(n)})} \mathcal{F}(\{h^{(\cdot)}\}) = \frac{\delta}{\delta(\mathfrak{a}_i^{(n)})} {}^k \mathcal{F}(\{\mathfrak{a}^{(\cdot)}\}) = {}^k \langle S_i^n \rangle. \quad (2.9)$$

For the sake of simplicity, we present relations between pair correlation functions for the BEG model (2.2) only. These relations can be obtained from (2.9) ($n = 1, 2$; $J = J^{(11)}$, $J' = J^{(22)}$, $J^{(12)} = J^{(21)} = 0$). Using matrix notations in the indices i, j and performing Fourier transformation, we get a system of four equations relating $\langle S^n S^m \rangle_{\vec{q}}^c$ and ${}^k \langle S^n S^m \rangle_{\vec{q}}^c$. In a matrix form it reads

$$\widehat{b}(\vec{q}) = {}^k \widehat{b}(\vec{q}) + {}^k \widehat{b}(\vec{q}) \begin{pmatrix} J_{\vec{q}} & 0 \\ 0 & J'_{\vec{q}} \end{pmatrix} \widehat{b}(\vec{q}), \quad (2.10)$$

$$\widehat{b}(\vec{q}) = \begin{pmatrix} \langle SS \rangle_{\vec{q}}^c & \langle SS^2 \rangle_{\vec{q}}^c \\ \langle S^2 S \rangle_{\vec{q}}^c & \langle S^2 S^2 \rangle_{\vec{q}}^c \end{pmatrix}; \quad {}^k \widehat{b}(\vec{q}) = \begin{pmatrix} {}^k \langle SS \rangle_{\vec{q}}^c & {}^k \langle SS^2 \rangle_{\vec{q}}^c \\ {}^k \langle S^2 S \rangle_{\vec{q}}^c & {}^k \langle S^2 S^2 \rangle_{\vec{q}}^c \end{pmatrix}. \quad (2.11)$$

From equation (2.10) one can easily find the pair CFs of the BEG model expressed in terms of pair CFs of the reference system, the long-range interactions taken into account in the MFA.

3. Two particle cluster approximation in short-range interactions

In this section we consider the reference pseudospin system with Hamiltonian (2.4). Let us divide the lattice into two-particle clusters. As $\sum_{n=1}^{\eta} {}^r \varphi_i^{(n)} S_i^n$ we denote an operator of the effective field created by the site r and acting on the site i , provided that the site r is a nearest neighbour of the site i ($r \in \pi_i$). Apparently, when the lattice is divided into the two-particle clusters, the number of fields acting on the given site is equal to the number of the nearest neighbours z . We transfer from summing over lattice sites to summing over clusters [22]:

$$\begin{aligned} \frac{1}{2} \sum_{i, \delta} K^{(nm)} S_i^n S_{i+\delta}^m &= \sum_{(1,2)} K^{(nm)} S_1^n S_2^m; \\ \sum_i \sum_{r \in \pi_i} {}^r \varphi_i^{(n)} S_i^n &= \sum_{(1,2)} \left({}^2 \varphi_1^{(n)} S_1^n + {}^1 \varphi_2^{(n)} S_2^n \right). \end{aligned} \quad (3.1)$$

Using (3.1), we can write the reference Hamiltonian (2.4) in the form

$${}^k \mathcal{H}(\{\mathfrak{a}^{(\cdot)}\}, \{\varphi^{(\cdot)}\}) = \sum_1 \mathcal{H}_1(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}) + \sum_{(1,2)} U_{12}, \quad (3.2)$$

provided that

$$\mathcal{H}_1(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}) = \sum_{n=1}^{\eta} \tilde{\mathfrak{a}}_1^{(n)} S_1^n; \quad \tilde{\mathfrak{a}}_1^{(n)} = \mathfrak{a}_1^{(n)} + \sum_{r \in \pi_1} {}^r \varphi_1^{(n)}, \quad (3.3)$$

$$U_{12} = \sum_{n=1}^{\eta} \left(-{}^2 \varphi_1^{(n)} S_1^n - {}^1 \varphi_2^{(n)} S_2^n + \sum_{m=1}^{\eta} K^{(nm)} S_1^n S_2^m \right). \quad (3.4)$$

Notation $\mathcal{H}_1(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\})$ means that $\mathcal{H}_1$ is a function of $(\tilde{\mathfrak{a}}_1^{(1)}, \dots, \tilde{\mathfrak{a}}_1^{(\eta)})$.

For ${}^k\mathcal{F}(\{\mathfrak{a}^{(\cdot)}\}, \{\varphi^{(\cdot)}\})$ we have:

$${}^k\mathcal{F}(\{\mathfrak{a}^{(\cdot)}\}, \{\varphi^{(\cdot)}\}) = \ln \text{Sp}_{\{S\}} \exp \left[{}^k\mathcal{H}(\{\mathfrak{a}^{(\cdot)}\}, \{\varphi^{(\cdot)}\}) \right] = \sum_1 F_1(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}) + \ln \langle \exp \left(\sum_{(1,2)} U_{12} \right) \rangle_{\rho_0}; \quad (3.5)$$

$$\langle A \rangle_{\rho_0} = \text{Sp}_{\{S\}} (\rho_0(\{S\}) \cdot A); \quad \rho_0(\{S\}) = \prod_1 \rho_1(S_1) = \prod_1 \frac{\exp(\mathcal{H}_1)}{Z_1}. \quad (3.6)$$

Here we introduced the following notations for the single-particle F_1 -function:

$$F_1(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}) = \ln Z_1(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}); \quad Z_1(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}) = \text{Sp}_{S_1} \exp [\mathcal{H}_1(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\})]. \quad (3.7)$$

Let us restrict ourselves to the first order of the cluster expansion [22]. Then ${}^k\mathcal{F}$ -function can be written as a sum of single-particle and two-particle intracluster F -functions

$${}^k\mathcal{F}(\{\mathfrak{a}^{(\cdot)}\}, \{\varphi^{(\cdot)}\}) = \sum_1 F_1(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}) + \sum_{(1,2)} \ln \langle \exp(U_{12}) \rangle_{\rho_0} = (1-z) \sum_1 F_1(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}) + \frac{1}{2} \sum_{1,2} F_{12}(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}, \{\tilde{\mathfrak{a}}_2^{(\cdot)}\}), \quad (3.8)$$

where the two-particle F_{12} -function reads:

$$F_{12}(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}, \{\tilde{\mathfrak{a}}_2^{(\cdot)}\}) = \ln Z_{12}(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}, \{\tilde{\mathfrak{a}}_2^{(\cdot)}\}) = \ln \text{Sp}_{S_1, S_2} \exp(\mathcal{H}_{12}), \quad (3.9)$$

$$\mathcal{H}_{12}(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}, \{\tilde{\mathfrak{a}}_2^{(\cdot)}\}) = \mathcal{H}_1(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}) + \mathcal{H}_2(\{\tilde{\mathfrak{a}}_2^{(\cdot)}\}) + U_{12} = \quad (3.10)$$

$$\sum_{n=1}^{\eta} \left({}^2\tilde{\mathfrak{a}}_1^{(n)} S_1^n + {}^1\tilde{\mathfrak{a}}_2^{(n)} S_2^n + \sum_{m=1}^{\eta} K^{(nm)} S_1^n S_2^m \right), \quad (3.11)$$

$${}^1\tilde{\mathfrak{a}}_2^{(n)} = \tilde{\mathfrak{a}}_2^{(n)} - {}^1\varphi_2^{(n)} = \mathfrak{a}_2^{(n)} + \sum_{\substack{r \in \pi_2 \\ r \neq 1}} {}^r\varphi_2^{(n)}.$$

Let us consider now the ${}^k\mathcal{F}$ -function. Using the method, proposed in [23] for the case $\eta = 1$ we can obtain equations for $\langle S_1^n \rangle = {}^k\langle S_1^n \rangle$ and cluster fields ${}^r\varphi_1^{(n)}$. From (2.8) and (2.9) we get:

$$\langle S_1^n \rangle = \frac{\partial {}^k\mathcal{F}}{\partial \mathfrak{a}_1^{(n)}} + \sum_i \sum_{r \in \pi_i} \sum_m \frac{\partial {}^k\mathcal{F}}{\partial {}^r\varphi_i^{(m)}} \cdot \frac{\delta {}^r\varphi_i^{(m)}}{\delta \mathfrak{a}_1^{(n)}}. \quad (3.12)$$

Taking into account the fact that ${}^k\mathcal{F}$ -function (3.8) is a sum of single-particle and two-particle F -functions and making use of the notations (3.3) and

(3.11), we get the following expressions for the partial derivatives of ${}^k\mathcal{F}$ -functions:

$$\frac{\partial {}^k\mathcal{F}}{\partial \mathfrak{a}_1^{(n)}} = (1-z) \cdot F_1 \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \right) + \sum_{r \in \pi_1} F_{1r} \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \right), \quad (3.13)$$

$$\frac{\partial {}^k\mathcal{F}}{\partial {}^r\varphi_i^{(n)}} = (1-z) \cdot F_i \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \right) + \sum_{r \in \pi_i} F_{ir} \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \right) - F_{ir_1} \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \right); \quad (r_1 \in \pi_i). \quad (3.14)$$

Here we use the notations for the partial derivatives of the single-particle and two-particle F -functions – the single-site and pair intracluster CFs:

$$F_i \left(\begin{smallmatrix} \nu_1 \\ n_1 \end{smallmatrix} \middle| \begin{smallmatrix} \nu_2 \\ n_2 \end{smallmatrix} \middle| \dots \begin{smallmatrix} \nu_k \\ n_k \end{smallmatrix} \middle| \{\tilde{\mathfrak{a}}_i^{(\cdot)}\} \right) = \frac{\partial^{\nu_1}}{\partial (\tilde{\mathfrak{a}}_i^{(n_1)})^{\nu_1}} \dots \frac{\partial^{\nu_k}}{\partial (\tilde{\mathfrak{a}}_i^{(n_k)})^{\nu_k}} F_i(\{\tilde{\mathfrak{a}}_i^{(\cdot)}\}), \quad (3.15)$$

$$F_{ir} \left(\begin{smallmatrix} \nu_1 \\ n_1 \end{smallmatrix} \middle| \begin{smallmatrix} \nu_2 \\ n_2 \end{smallmatrix} \middle| \dots \begin{smallmatrix} \nu_k \\ n_k \end{smallmatrix} \middle| \begin{smallmatrix} \mu_1 \\ m_1 \end{smallmatrix} \middle| \begin{smallmatrix} \mu_2 \\ m_2 \end{smallmatrix} \middle| \dots \begin{smallmatrix} \mu_l \\ m_l \end{smallmatrix} \middle| \{^r\tilde{\mathfrak{a}}_i^{(\cdot)}\}, \{^i\tilde{\mathfrak{a}}_r^{(\cdot)}\} \right) = \frac{\partial^{\nu_1}}{\partial ({}^r\tilde{\mathfrak{a}}_i^{(n_1)})^{\nu_1}} \dots \frac{\partial^{\nu_k}}{\partial ({}^r\tilde{\mathfrak{a}}_i^{(n_k)})^{\nu_k}} \frac{\partial^{\mu_1}}{\partial ({}^i\tilde{\mathfrak{a}}_r^{(m_1)})^{\mu_1}} \dots \frac{\partial^{\mu_l}}{\partial ({}^i\tilde{\mathfrak{a}}_r^{(m_l)})^{\mu_l}} F_{ir}(\{^r\tilde{\mathfrak{a}}_i^{(\cdot)}\}, \{^i\tilde{\mathfrak{a}}_r^{(\cdot)}\}), \quad (3.16)$$

On the basis of (2.9), (3.3), (3.11), (3.12), (3.13) and (3.14) taking into account the condition of an extremum of ${}^k\mathcal{F}$ -function with respect to ${}^r\varphi_i^{(n)}$

$$\frac{\partial {}^k\mathcal{F}}{\partial {}^r\varphi_i^{(n)}} = 0, \quad (3.17)$$

we can easily get the system of $(z+1)\eta N$ equations for ${}^r\varphi_i^{(n)}$ and $\langle S_i^n \rangle$ ($n = 1, \dots, \eta$; $i = 1, \dots, N$).

$$\langle S_1^n \rangle = F_1 \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \{\tilde{\mathfrak{a}}_1^{(\cdot)}\} \right) \quad (3.18)$$

$$F_1 \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \{\tilde{\mathfrak{a}}_1^{(\cdot)}\} \right) = F_{1r} \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \{^r\tilde{\mathfrak{a}}_1^{(\cdot)}\}, \{^1\tilde{\mathfrak{a}}_r^{(\cdot)}\} \right) \quad (3.19)$$

On the other hand, from (3.7), (3.9), and definitions of intracluster averages

$$\langle A \rangle_{\rho_1} = \text{Sp}_{S_1} [\rho_1(S_1) \cdot A] \quad ; \quad \langle A \rangle_{\rho_{1r}} = \text{Sp}_{S_1, S_r} [\rho_{1r}(S_1, S_r) \cdot A] \quad , \quad (3.20)$$

we obtain the relations for the single-site intracluster CFs

$$F_1 \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \right) = \langle S_1^n \rangle_{\rho_1} \quad ; \quad F_{1r} \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \right) = \langle S_1^n \rangle_{\rho_{1r}}, \quad (3.21)$$

the quantities are averaged with the intracluster single-particle and two-particle density matrices

$$\rho_1(S_1) = \frac{\exp \left[\mathcal{H}_1(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\}) \right]}{Z_1(\{\tilde{\mathfrak{a}}_1^{(\cdot)}\})}; \quad (3.22)$$

$$\rho_{1r}(S_1, S_r) = \frac{\exp \left[\mathcal{H}_{1r}(\{^r\tilde{\mathfrak{a}}_1^{(\cdot)}\}, \{^1\tilde{\mathfrak{a}}_r^{(\cdot)}\}) \right]}{Z_{1r}(\{^r\tilde{\mathfrak{a}}_1^{(\cdot)}\}, \{^1\tilde{\mathfrak{a}}_r^{(\cdot)}\})}.$$

Hence, from the condition of ${}^k\mathcal{F}$ -function extremum we have derived (see (3.18), (3.19)) the system of $z\eta N$ equations

$$\langle S_1^n \rangle_{\rho_1} = \langle S_1^n \rangle_{\rho_{1r}} ; \quad (n=1, \dots, \eta) . \quad (3.23)$$

As can be seen from definition (3.20), the system of $z\eta N$ equations (3.23) is equivalent to $z\eta N$ independent relations between the density matrices

$$\rho_1(S_1) = \text{Sp}_{S_r}[\rho_{1r}(S_1, S_r)] ; \quad S = (-\eta, -\eta + 2, \dots, \eta - 2, \eta) . \quad (3.24)$$

Among $z(\eta + 1)N$ relations (3.24), only $z\eta N$ are independent, for zN conditions $\rho_1(S_1)$, $\rho_{1r}(S_1, S_r)$ are obeyed identically as follows from the form of $\text{Sp}_{S_1}[\rho_1(S_1)] = \text{Sp}_{S_1, S_r}[\rho_{1r}(S_1, S_r)] = 1$. Hence, in the TPCA, the condition of ${}^k\mathcal{F}$ -function extremum yields the relations (3.24) between the intracluster density matrices.

Let us note that in uniform fields $h_i^{(n)}$ ($h_i^{(n)} = h^{(n)}$, $\langle S_i^n \rangle = \langle S^n \rangle$, $\mathfrak{a}_i^{(n)} = \mathfrak{a}^{(n)}$), that is, when

$$\begin{aligned} {}^r\tilde{\mathfrak{a}}_1^{(n)} &= \tilde{\mathfrak{a}}^{(n)} = \mathfrak{a}^{(n)} + (z - 1)\varphi^{(n)} ; \quad \tilde{\mathfrak{a}}_1^{(n)} = \tilde{\mathfrak{a}}^{(n)} = \mathfrak{a}^{(n)} + z\varphi^{(n)} ; \quad (3.25) \\ \mathfrak{a}^{(n)} &= h^{(n)} + \sum_{m=1}^{\eta} J_0^{(nm)} \langle S^m \rangle ; \quad J_0^{(nm)} = J^{(nm)}(\vec{q} = 0) , \end{aligned}$$

relations (3.18) and (3.19) form the system of 2η equations for $\varphi^{(n)}$ and $\langle S^n \rangle$. When the long-range interactions are absent ($J_0^{(nm)} = 0$) and the fields are uniform, we have the system of η equations (3.19) for the cluster fields $\varphi^{(n)}$ and η expressions (3.18) for the single-site CFs $\langle S^n \rangle$.

Let us briefly consider the proposed by us [3] method of calculation of pair CFs of the reference system with an arbitrary value of η , which is based on the method developed in [23] for the case $\eta = 1$. From (2.8) and (3.18) one can obtain an expression for pair CFs of the reference system

$${}^kb_{12}^{(nm)} = {}^k\langle S_1^n S_2^m \rangle^c = \sum_{k=1}^{\eta} F_1 \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \begin{smallmatrix} 1 \\ k \end{smallmatrix} \right) \cdot \frac{\delta \tilde{\mathfrak{a}}_1^{(k)}}{\delta \mathfrak{a}_2^{(m)}} . \quad (3.26)$$

Since evaluation of $F_1 \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \begin{smallmatrix} 1 \\ k \end{smallmatrix} \right)$ for a particular system is straightforward, we only have to find an equation for $\delta \tilde{\mathfrak{a}}_1^{(k)} / \delta \mathfrak{a}_2^{(m)}$.

Let us introduce the notations

$$\frac{\delta \tilde{\mathfrak{a}}_1^{(k)}}{\delta \mathfrak{a}_2^{(m)}} = \tilde{\mathfrak{a}}_{12}(k|m) ; \quad \frac{\delta {}^r\tilde{\mathfrak{a}}_1^{(k)}}{\delta \mathfrak{a}_2^{(m)}} = {}^r\tilde{\mathfrak{a}}_{12}(k|m) ; \quad \frac{\delta {}^r\varphi_1^{(k)}}{\delta \mathfrak{a}_2^{(m)}} = {}^r\varphi_{12}(k|m) . \quad (3.27)$$

Differentiating both sides of equation (3.19) with respect to $\mathfrak{a}_2^{(m)}$, and taking into account the relation

$${}^r\tilde{\mathfrak{a}}_{12}(k|m) = \tilde{\mathfrak{a}}_{12}(k|m) - {}^r\varphi_{12}(k|m) \quad (3.28)$$

(see (3.11)), we get

$$\begin{aligned} \sum_{k=1}^{\eta} F_1 \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \begin{smallmatrix} 1 \\ k \end{smallmatrix} \right) \cdot \tilde{\mathfrak{a}}_{12}(k|m) &= \sum_{k=1}^{\eta} F_{1r} \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \begin{smallmatrix} 1 \\ k \end{smallmatrix} \right) \left[\tilde{\mathfrak{a}}_{12}(k|m) - {}^r\varphi_{12}(k|m) \right] + \\ &\quad \sum_{k=1}^{\eta} F_{1r} \left(\begin{smallmatrix} 1 \\ n \end{smallmatrix} \middle| \begin{smallmatrix} 1 \\ k \end{smallmatrix} \right) \left[\tilde{\mathfrak{a}}_{r2}(k|m) - {}^1\varphi_{r2}(k|m) \right] , \quad (3.29) \end{aligned}$$

which can be transformed to

$$\left[\widehat{F}_{1r}^{(20)} + \widehat{F}_1^{(2)} \right] \cdot \widehat{\mathfrak{a}}_{12} + \widehat{F}_{1r}^{(11)} \cdot \widehat{\mathfrak{a}}_{r2} = \widehat{F}_{1r}^{(20)} \cdot {}^r\widehat{\varphi}_{12} + \widehat{F}_{1r}^{(11)} \cdot {}^1\widehat{\varphi}_{r2} . \quad (3.30)$$

Here we use the notations:

$$\begin{aligned} \widehat{F}_i^{(2)} &= \begin{pmatrix} F_i \left(\begin{smallmatrix} 2 \\ 1 \end{smallmatrix} \middle| \right) & F_i \left(\begin{smallmatrix} 1 & 1 \\ 1 & 2 \end{smallmatrix} \middle| \right) & \dots & F_i \left(\begin{smallmatrix} 1 & 1 \\ 1 & \eta \end{smallmatrix} \middle| \right) \\ \vdots & & & \\ F_i \left(\begin{smallmatrix} 1 & 1 \\ \eta & 1 \end{smallmatrix} \middle| \right) & F_i \left(\begin{smallmatrix} 1 & 1 \\ \eta & 2 \end{smallmatrix} \middle| \right) & \dots & F_i \left(\begin{smallmatrix} 2 \\ \eta \end{smallmatrix} \middle| \right) \end{pmatrix} , \quad (3.31) \\ \widehat{F}_{ir}^{(20)} &= \begin{pmatrix} F_{ir} \left(\begin{smallmatrix} 2 \\ 1 \end{smallmatrix} \middle| \right) & F_{ir} \left(\begin{smallmatrix} 1 & 1 \\ 1 & 2 \end{smallmatrix} \middle| \right) & \dots & F_{ir} \left(\begin{smallmatrix} 1 & 1 \\ 1 & \eta \end{smallmatrix} \middle| \right) \\ \vdots & & & \\ F_{ir} \left(\begin{smallmatrix} 1 & 1 \\ \eta & 1 \end{smallmatrix} \middle| \right) & F_{ir} \left(\begin{smallmatrix} 1 & 1 \\ \eta & 2 \end{smallmatrix} \middle| \right) & \dots & F_{ir} \left(\begin{smallmatrix} 2 \\ \eta \end{smallmatrix} \middle| \right) \end{pmatrix} , \\ \widehat{F}_{ir}^{(11)} &= \begin{pmatrix} F_{ir} \left(\begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix} \middle| \right) & \dots & F_{ir} \left(\begin{smallmatrix} 1 & 1 \\ 1 & \eta \end{smallmatrix} \middle| \right) \\ \vdots & & \\ F_{ir} \left(\begin{smallmatrix} 1 & 1 \\ \eta & 1 \end{smallmatrix} \middle| \right) & \dots & F_{ir} \left(\begin{smallmatrix} 1 & 1 \\ \eta & \eta \end{smallmatrix} \middle| \right) \end{pmatrix} , \\ \widehat{\mathfrak{a}}_{ir} &= \begin{pmatrix} \mathfrak{a}_{ir}(1|1) & \dots & \mathfrak{a}_{ir}(1|\eta) \\ \vdots & & \\ \mathfrak{a}_{ir}(\eta|1) & \dots & \mathfrak{a}_{ir}(\eta|\eta) \end{pmatrix} . \end{aligned}$$

Let us note that equations (3.30) contain unknown variables ${}^r\widehat{\varphi}_{12}$ and ${}^1\widehat{\varphi}_{r2}$, for which we need to derive an independent equation. Using the relations

$$F_1 \left(\begin{smallmatrix} 2 \\ n \end{smallmatrix} \middle| \right) = F_{1r} \left(\begin{smallmatrix} 2 \\ n \end{smallmatrix} \middle| \right) ; \quad F_1 \left(\begin{smallmatrix} 1 & 1 \\ n & m \end{smallmatrix} \middle| \right) = F_{1r} \left(\begin{smallmatrix} 1 & 1 \\ n & m \end{smallmatrix} \middle| \right) , \quad (3.32)$$

following from the relations between the density matrices (3.24) and introducing the notations

$$\widehat{f}_{1r} = \left[\widehat{F}_{1r}^{(20)} \right]^{-1} \cdot \widehat{F}_{1r}^{(11)} , \quad (3.33)$$

we rewrite (3.30) in the form

$${}^r\widehat{\varphi}_{12} + \widehat{f}_{1r} \cdot {}^1\widehat{\varphi}_{r2} = \widehat{f}_{1r} \cdot \widehat{\mathfrak{a}}_{r2} . \quad (3.34)$$

Exchanging indices $r \rightleftharpoons 1$, we obtain

$$\widehat{f}_{r1} \cdot {}^r\widehat{\varphi}_{12} + {}^1\widehat{\varphi}_{r2} = \widehat{f}_{r1} \cdot \widehat{\mathfrak{a}}_{12} . \quad (3.35)$$

(3.34) and (3.35) are the system of equations for ${}^r\widehat{\varphi}_{12}$ and ${}^1\widehat{\varphi}_{r2}$. Carrying out summation over $r \in \pi_1$ in (3.34) and considering the fact that

$$\sum_{r \in \pi_1} {}^r\widehat{\varphi}_{12} = \widehat{\mathfrak{a}}_{12} - \widehat{\mathfrak{a}}_{12} = \widehat{\mathfrak{a}}_{12} - \delta_{12} \cdot \widehat{1} , \quad (3.36)$$

we can obtain from (3.34), (3.35) a closed equation for $\widehat{\mathfrak{a}}_{12}$.

$$\widehat{Q}_{11} \cdot \widehat{\mathfrak{a}}_{12} = \delta_{12} \cdot \widehat{1} + \sum_{r \in \pi_1} \widehat{f}_{1r} \cdot \widehat{d}_{r1}^{-1} \cdot \widehat{\mathfrak{a}}_{r2} \cdot \pi_{1r} \quad (3.37)$$

Here we use the notations:

$$\widehat{Q}_{11} = \widehat{1} + \sum_{r \in \pi_1} \widehat{f}_{1r} \cdot \widehat{d}_{r1r}^{-1} \cdot \widehat{f}_{r1} ; \quad \widehat{d}_{r1r} = \widehat{1} - \widehat{f}_{r1} \cdot \widehat{f}_{1r} ; \quad \pi_{1r} = \begin{cases} 1, & r \in \pi_1 \\ 0, & r \notin \pi_1 \end{cases}. \quad (3.38)$$

In uniform fields the following relations hold:

$$\widehat{\mathfrak{a}}_{12} = \widehat{\mathfrak{a}}_{(1-2)} ; \quad \widehat{f}_{1r} = \widehat{f}_{(1-r)} = \widehat{f} ; \quad \widehat{d}_{r1r} = \widehat{d}_{(1-r)} = \widehat{d} = \widehat{1} - \widehat{f}^2. \quad (3.39)$$

Performing in (3.37) a Fourier transformation, the fields being uniform, and solving the obtained equation, we find $\widehat{\mathfrak{a}}(\vec{q})$

$$\widehat{\mathfrak{a}}(\vec{q}) = \left[z \cdot \widehat{1} - (z-1)(\widehat{1} + \widehat{f}) + z(\widehat{1} - \widehat{f})^{-1} \cdot \widehat{f} \cdot \Theta(\vec{q}) \right]^{-1} \cdot (\widehat{1} + \widehat{f}), \quad (3.40)$$

where for a hypercubic lattice

$$\Theta(\vec{q}) = 1 - \frac{\pi(\vec{q})}{z} = \frac{2}{d} \sum_{i=1}^d \sin^2 \left(\frac{q_i \cdot a}{2} \right). \quad (3.41)$$

$d = z/2$ is the lattice dimension, $\pi(\vec{q})$ is the Fourier transform of π_{1r} .

Using the matrix form of (3.26) and performing a Fourier transformation, taking into account (3.40), we get the following relation for pair CFs of the reference system

$$\begin{aligned} {}^k \widehat{b}(\vec{q}) = \widehat{F}_1^{(2)} \cdot \widehat{\mathfrak{a}}(\vec{q}) &= \frac{1}{z} \left[\left(\widehat{F}^{(+)} \right)^{-1} + \left(\frac{1}{z} - 1 \right) \left(\widehat{F}^{(2)} \right)^{-1} + \right. \\ &\quad \left. \left(\widehat{F}^{(+)} \right)^{-1} \left\{ \widehat{F}^{(2)} \cdot \left(\widehat{F}^{(-)} \right)^{-1} - \widehat{1} \right\} \Theta(\vec{q}) \right]^{-1}, \end{aligned} \quad (3.42)$$

where $\widehat{F}^{(+)} = \widehat{F}^{(2)} + \widehat{F}^{(11)}$, $\widehat{F}^{(-)} = \widehat{F}^{(2)} - \widehat{F}^{(11)}$.

4. The Blume-Emery-Griffiths model

Let us consider the reference Blume-Emery-Griffiths model ($\eta = 2$), which is described by the Hamiltonian

$${}^k \mathcal{H}(\{\mathfrak{a}\}, \{\mathfrak{a}'\}) = \beta \sum_{i=1}^N [\mathfrak{a}_i S_i + \mathfrak{a}'_i S_i^2] + \frac{1}{2} \beta \sum_{i,\delta} [K S_i S_{i+\delta} + K' S_i^2 S_{i+\delta}^2]. \quad (4.1)$$

Here $\mathfrak{a}_i = \Gamma_i + \sum_{j=1}^N J_{ij} \langle S_j \rangle$, $\mathfrak{a}'_i = D_i + \sum_{j=1}^N J'_{ij} \langle S_j^2 \rangle$, Γ_i is an external field. D_i stands for single-ion anisotropy. Let us note that the factor $\beta = (k_B T)^{-1}$ is written explicitly hereafter.

On the basis of (3.3), (3.7) and (3.9), (3.10) we calculate the single-particle and two-particle F -functions

$$F_1(T, \tilde{\mathfrak{a}}_1, \tilde{\mathfrak{a}}'_1) = \ln \left(2 \exp(4\beta \tilde{\mathfrak{a}}'_1) \cdot \text{ch}(2\beta \tilde{\mathfrak{a}}_1) + 1 \right), \quad (4.2)$$

$$\begin{aligned} F_{12}(T, {}^2 \tilde{\mathfrak{a}}_1, {}^2 \tilde{\mathfrak{a}}'_1, {}^1 \tilde{\mathfrak{a}}_2, {}^1 \tilde{\mathfrak{a}}'_2) &= \ln \left\{ 2 \exp[4\beta({}^2 \tilde{\mathfrak{a}}'_1 + {}^1 \tilde{\mathfrak{a}}'_2 + 4K')] \times \right. \\ &\quad \left(\exp(4\beta K) \cdot \text{ch}[2\beta({}^2 \tilde{\mathfrak{a}}_1 + {}^1 \tilde{\mathfrak{a}}_2)] + \exp(-4\beta K) \cdot \text{ch}[2\beta({}^2 \tilde{\mathfrak{a}}_1 - {}^1 \tilde{\mathfrak{a}}_2)] \right) + \\ &\quad \left. 2 \exp(4\beta {}^2 \tilde{\mathfrak{a}}'_1) \cdot \text{ch}(2\beta {}^2 \tilde{\mathfrak{a}}_1) + 2 \exp(4\beta {}^1 \tilde{\mathfrak{a}}'_2) \cdot \text{ch}(2\beta {}^1 \tilde{\mathfrak{a}}_2) + 1 \right\}. \end{aligned} \quad (4.3)$$

In uniform fields, that is, when the relations

$$\begin{aligned}\tilde{\mathfrak{a}}_1 &= \tilde{\mathfrak{a}} = \mathfrak{a} + z \cdot \varphi ; & {}^r \tilde{\mathfrak{a}}_1 &= \tilde{\mathfrak{a}} = \mathfrak{a} + (z - 1)\varphi ; \\ \tilde{\mathfrak{a}}'_1 &= \tilde{\mathfrak{a}}' = \mathfrak{a}' + z \cdot \varphi' ; & {}^r \tilde{\mathfrak{a}}'_1 &= \tilde{\mathfrak{a}}' = \mathfrak{a}' + (z - 1)\varphi'\end{aligned}\quad (4.4)$$

hold, we have

$$\begin{aligned}\frac{1}{N} {}^k \mathcal{F}(T, \Gamma, D, \varphi, \varphi', \langle S \rangle, \langle S^2 \rangle) &= (1 - z)F_1(T, \tilde{\mathfrak{a}}, \tilde{\mathfrak{a}}') + \frac{z}{2}F_{12}(T, \tilde{\mathfrak{a}}, \tilde{\mathfrak{a}}'); \\ F_1(T, \tilde{\mathfrak{a}}, \tilde{\mathfrak{a}}') &= \ln Z_1(T, \tilde{\mathfrak{a}}, \tilde{\mathfrak{a}}') ; & F_{12}(T, \tilde{\mathfrak{a}}, \tilde{\mathfrak{a}}') &= \ln Z_{12}(T, \tilde{\mathfrak{a}}, \tilde{\mathfrak{a}}') ; \\ Z_1(T, \tilde{\mathfrak{a}}, \tilde{\mathfrak{a}}') &= 2e^{4\beta\tilde{\mathfrak{a}}'} \cdot \text{ch}(2\beta\tilde{\mathfrak{a}}) + 1 ; \\ Z_{12}(T, \tilde{\mathfrak{a}}, \tilde{\mathfrak{a}}') &= 2e^{8\beta(\tilde{\mathfrak{a}}' + 2K')} \left(e^{4\beta K} \cdot \text{ch}(4\beta\tilde{\mathfrak{a}}) + e^{-4\beta K} \right) + \\ &\quad 4e^{4\beta\tilde{\mathfrak{a}}'} \cdot \text{ch}(2\beta\tilde{\mathfrak{a}}) + 1 .\end{aligned}\quad (4.5)$$

Let us note that if $J = J' = 0$ the dependence ${}^k \mathcal{F} = {}^k \mathcal{F}(T, \Gamma, D, \varphi, \varphi')$ takes place. To obtain an explicit system of equations for the cluster fields φ, φ' , single-site CFs $\langle S \rangle, \langle S^2 \rangle$ and expressions for pair CFs, we need to know intracluster CFs $F_1(\begin{smallmatrix} 1 \\ n \end{smallmatrix} |), F_1(\begin{smallmatrix} 2 \\ n \end{smallmatrix} |), F_1(\begin{smallmatrix} 1 & 1 \\ n & m \end{smallmatrix} |), F_{1r}(\begin{smallmatrix} 1 \\ n \end{smallmatrix} |), F_{1r}(\begin{smallmatrix} 2 \\ n \end{smallmatrix} |), F_{1r}(\begin{smallmatrix} 1 & 1 \\ n & m \end{smallmatrix} |)$. Differentiating F -functions with respect to relevant variables ($n, m = 1$ and $n, m = 2$ correspond to differentiation to single-particle F_1 -function with respect to $\tilde{\mathfrak{a}}_1$ and $\tilde{\mathfrak{a}}'_1$ (see (3.15)) and of two-particle F_{12} -function with respect to ${}^2\tilde{\mathfrak{a}}_1$ and ${}^2\tilde{\mathfrak{a}}'_1$, or ${}^1\tilde{\mathfrak{a}}_2$ and ${}^1\tilde{\mathfrak{a}}'_2$ (see (3.16))) and going to the uniform fields case, we obtain

$$\begin{aligned}F_1(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix} |) &= 4e^{4\beta\tilde{\mathfrak{a}}'} \cdot \text{sh}(2\beta\tilde{\mathfrak{a}}) \cdot Z_1^{-1} ; \\ F_1(\begin{smallmatrix} 1 \\ 2 \end{smallmatrix} |) &= 8e^{4\beta\tilde{\mathfrak{a}}'} \cdot \text{ch}(2\beta\tilde{\mathfrak{a}}) \cdot Z_1^{-1} ; \\ F_1(\begin{smallmatrix} 2 \\ 1 \end{smallmatrix} |) &= 8e^{4\beta\tilde{\mathfrak{a}}'} \left[2e^{4\beta\tilde{\mathfrak{a}}'} + \text{ch}(2\beta\tilde{\mathfrak{a}}) \right] Z_1^{-2} ; \\ F_1(\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} |) &= 32e^{4\beta\tilde{\mathfrak{a}}'} \cdot \text{ch}(2\beta\tilde{\mathfrak{a}}) \cdot Z_1^{-2} ; \\ F_1(\begin{smallmatrix} 1 & 1 \\ 2 & 1 \end{smallmatrix} |) &= F_1(\begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix} |) = 16e^{4\beta\tilde{\mathfrak{a}}'} \cdot \text{sh}(2\beta\tilde{\mathfrak{a}}) \cdot Z_1^{-2} ; \\ F_{12}(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix} |) &= 4 \left(e^{4\beta(2\tilde{\mathfrak{a}}' + 4K' + K)} \cdot \text{sh}(4\beta\tilde{\mathfrak{a}}) + e^{4\beta\tilde{\mathfrak{a}}'} \cdot \text{sh}(2\beta\tilde{\mathfrak{a}}) \right) \cdot Z_{12}^{-1} ; \\ F_{12}(\begin{smallmatrix} 1 \\ 2 \end{smallmatrix} |) &= 8 \left\{ e^{8\beta(\tilde{\mathfrak{a}}' + 2K')} \left[e^{4\beta K} \cdot \text{ch}(4\beta\tilde{\mathfrak{a}}) + e^{-4\beta K} \right] + \right. \\ &\quad \left. e^{4\beta\tilde{\mathfrak{a}}'} \cdot \text{ch}(2\beta\tilde{\mathfrak{a}}) \right\} \cdot Z_{12}^{-1} ; \\ F_{12}(\begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix} |) &= 8e^{8\beta\tilde{\mathfrak{a}}'} \left\{ e^{16\beta K'} \left[4e^{8\beta(\tilde{\mathfrak{a}}' + 2K')} \cdot \text{sh}(8\beta K) + \right. \right. \\ &\quad \left. 8e^{4\beta\tilde{\mathfrak{a}}'} \cdot \text{sh}(4\beta K) \cdot \text{ch}(2\beta\tilde{\mathfrak{a}}) + \right. \\ &\quad \left. e^{4\beta K} \cdot \text{ch}(4\beta\tilde{\mathfrak{a}}) - e^{-4\beta K} \right] - 2\text{sh}^2(2\beta\tilde{\mathfrak{a}}) \left. \right\} \cdot Z_{12}^{-2} ; \\ F_{12}(\begin{smallmatrix} 1 & 1 \\ 2 & 2 \end{smallmatrix} |) &= 32e^{8\beta\tilde{\mathfrak{a}}'} \left\{ e^{16\beta K'} \left[e^{4\beta K} \cdot \text{ch}(4\beta\tilde{\mathfrak{a}}) + e^{-4\beta K} \right] - \right. \\ &\quad \left. 2\text{ch}^2(2\beta\tilde{\mathfrak{a}}) \right\} \cdot Z_{12}^{-2} ; \\ F_{12}(\begin{smallmatrix} 1 & 1 \\ 1 & 2 \end{smallmatrix} |) &= F_{12}(\begin{smallmatrix} 1 & 1 \\ 2 & 1 \end{smallmatrix} |) = 16e^{8\beta\tilde{\mathfrak{a}}'} \left\{ 4e^{4\beta(\tilde{\mathfrak{a}}' + 4K')} \cdot \text{sh}(2\beta\tilde{\mathfrak{a}}) \cdot \text{sh}(4\beta K) + \right. \\ &\quad \left. e^{4\beta(4K' + K)} \cdot \text{sh}(4\beta\tilde{\mathfrak{a}}) - 2\text{sh}(2\beta\tilde{\mathfrak{a}}) \cdot \text{ch}(2\beta\tilde{\mathfrak{a}}) \right\} \cdot Z_{12}^{-2} .\end{aligned}\quad (4.7)$$

On the basis of (3.18), (3.19) and (4.7), (4.8) we can write an explicit system of equations for φ , φ' , $\langle S \rangle$, $\langle S^2 \rangle$ in the uniform fields case:

$$\langle S \rangle = \frac{4e^{4\beta\tilde{\alpha}'} \cdot \text{sh}(2\beta\tilde{\alpha})}{Z_1(T, \tilde{\alpha}, \tilde{\alpha}')} ; \quad \langle S^2 \rangle = \frac{8e^{4\beta\tilde{\alpha}'} \cdot \text{ch}(2\beta\tilde{\alpha})}{Z_1(T, \tilde{\alpha}, \tilde{\alpha}')} ; \quad (4.9)$$

$$\frac{e^{4\beta\tilde{\alpha}'} \cdot \text{sh}(2\beta\tilde{\alpha})}{Z_1(T, \tilde{\alpha}, \tilde{\alpha}')} = \frac{e^{4\beta(2\tilde{\alpha}'+4K'+K)} \cdot \text{sh}(4\beta\tilde{\alpha}) + e^{4\beta\tilde{\alpha}'} \cdot \text{sh}(2\beta\tilde{\alpha})}{Z_{12}(T, \tilde{\alpha}, \tilde{\alpha}')} ; \quad (4.10)$$

$$\frac{e^{4\beta\tilde{\alpha}'} \cdot \text{ch}(2\beta\tilde{\alpha})}{Z_1(T, \tilde{\alpha}, \tilde{\alpha}')} = \frac{e^{8\beta(\tilde{\alpha}'+2K')} \left[e^{4\beta K} \cdot \text{ch}(4\beta\tilde{\alpha}) + e^{-4\beta K} \right] + e^{4\beta\tilde{\alpha}'} \cdot \text{ch}(2\beta\tilde{\alpha})}{Z_{12}(T, \tilde{\alpha}, \tilde{\alpha}')} .$$

Let us note, that when long-range interactions are absent ($J = J' = 0$) we obtain the system of equations (4.10) for the cluster fields φ , φ' and expressions (4.9) for $\langle S \rangle$, $\langle S^2 \rangle$ (expressions (4.9) and the system of equations (4.10) are in agreement with the results of constant coupling approximation [17]).

On the basis of (3.42) ($\eta = 2$), considering the fact that $F_1(\begin{smallmatrix} 1 & 1 \\ 1 & 2 \end{smallmatrix}) = F_1(\begin{smallmatrix} 1 & 1 \\ 2 & 1 \end{smallmatrix})$, $F_{12}(\begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix}) = F_{12}(\begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix})$, we can obtain expressions for pair CFs of the reference BEG model.

$${}^k\hat{b}(\vec{q}) = \begin{pmatrix} {}^k\langle SS \rangle_{\vec{q}}^c & {}^k\langle SS^2 \rangle_{\vec{q}}^c \\ {}^k\langle S^2 S \rangle_{\vec{q}}^c & {}^k\langle S^2 S^2 \rangle_{\vec{q}}^c \end{pmatrix} = \frac{d^+ d^- d^{(2)}}{z(\tilde{b}_1 \tilde{b}_3 - (\tilde{b}_2)^2)} \cdot \begin{pmatrix} \tilde{b}_1 & \tilde{b}_2 \\ \tilde{b}_2 & \tilde{b}_3 \end{pmatrix} , \quad (4.11)$$

where

$$\tilde{b}_\alpha = d^{(-)} \left\{ d^{(2)} F_\alpha^{(+)} + \left(\frac{1}{z} - 1 \right) d^{(+)} F_\alpha^{(2)} \right\} - \quad (4.12)$$

$$d^{(2)} \left\{ F_\alpha^{(+)} \left(d^{(-)} + F_2^{(-)} F_2^{(2)} \right) - B_\alpha \right\} \Theta(\vec{q}) , \quad (\alpha=1,2,3) ;$$

$$\hat{F}^{(\xi)} = \begin{pmatrix} F_1^{(\xi)} & F_2^{(\xi)} \\ F_2^{(\xi)} & F_3^{(\xi)} \end{pmatrix} , \quad (\xi=+, -, 2) ; \quad \hat{F}^{(\pm)} = \hat{F}^{(2)} \pm \hat{F}^{(11)} ; \quad (4.13)$$

$$d^{(-)} = \det \left| \hat{F}^{(-)} \right| ; \quad d^{(+)} = \det \left| \hat{F}^{(+)} \right| ; \quad d^{(2)} = \det \left| \hat{F}^{(2)} \right| ;$$

$$\hat{F}^{(2)} = \begin{pmatrix} F_1(\begin{smallmatrix} 2 \\ 1 \end{smallmatrix}) & F_1(\begin{smallmatrix} 1 & 1 \\ 2 & 2 \end{smallmatrix}) \\ F_1(\begin{smallmatrix} 1 & 1 \\ 2 & 2 \end{smallmatrix}) & F_1(\begin{smallmatrix} 1 & 1 \\ 2 & 2 \end{smallmatrix}) \end{pmatrix} ; \quad \hat{F}^{(11)} = \begin{pmatrix} F_{12}(\begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix}) & F_{12}(\begin{smallmatrix} 1 & 1 \\ 2 & 2 \end{smallmatrix}) \\ F_{12}(\begin{smallmatrix} 1 & 1 \\ 2 & 2 \end{smallmatrix}) & F_{12}(\begin{smallmatrix} 1 & 1 \\ 2 & 2 \end{smallmatrix}) \end{pmatrix} ; \quad (4.14)$$

$$B_1 = F_1^{(+)} F_1^{(-)} F_3^{(2)} + F_2^{(+)} F_2^{(-)} F_1^{(2)} - F_2^{(+)} F_1^{(-)} F_2^{(2)} ; \quad (4.15)$$

$$B_2 = F_2^{(+)} F_1^{(-)} F_3^{(2)} + F_3^{(+)} F_2^{(-)} F_1^{(2)} - F_3^{(+)} F_1^{(-)} F_2^{(2)} ;$$

$$B_3 = F_3^{(+)} F_3^{(-)} F_1^{(2)} + F_2^{(+)} F_2^{(-)} F_3^{(2)} - F_2^{(+)} F_3^{(-)} F_2^{(2)} .$$

5. Numerical analysis results

In this section we discuss the results of numerical calculations ($\Gamma = 0$) of thermodynamic characteristics and pair correlation functions (at $\vec{q} = 0$) of BEG model on a simple cubic lattice ($z = 6$).

Here we use the following notations for the relative quantities:

$$t = \frac{3}{8} \frac{k_B T}{zK} , \quad d = \frac{\alpha'}{K} , \quad k' = \frac{4K'}{K} , \quad m = \frac{1}{2} \langle S \rangle , \quad q = \frac{1}{4} \langle S^2 \rangle ,$$

$$G_{11} = \frac{1}{4} \langle SS \rangle_{\vec{q}=0}^c , \quad G_{12} = \frac{1}{8} \langle SS^2 \rangle_{\vec{q}=0}^c , \quad G_{11} = \frac{1}{16} \langle S^2 S^2 \rangle_{\vec{q}=0}^c ;$$

and the terminology of [17]:

F – the ferromagnetic phase ($m \neq 0, q \neq \frac{2}{3}$),

P – the paramagnetic phase ($m = 0, q \neq \frac{2}{3}, q(t = \infty) = \frac{2}{3}$),

Q – the quadrupolar phase ($m = 0, q \neq \frac{2}{3}$).

In the two-particle cluster approximation the system of equations for φ, φ' (4.10) has several solutions, the number of which depends on values of parameters d, k' and temperature. Solution corresponding to **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 **F**-phase and **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 at $d < 0, k' > -0.1$ [17] and $d > 0, k' > -1 - \frac{1}{6}d$ (see figure 1) consists of seven regions:

I – the phase transition **Q** $\leftrightarrow$ **P** of the first order (**QP1**),

II – the PT **FP2**,

III – the PT **FP1**,

IV – the PT is absent,

V – the PTs **QF1** and **FP2**,

VI – the PTs **QF1** and **FP1**,

VII – the PTs **FQ1** and **QP1**.

In the present paper we restrict our consideration to the regions $d < 0, k' > -0.1$ and $d > 0, k' > -1 - \frac{1}{6}d$, since for the regions $d > 0, k' < -1 - \frac{1}{6}d$ and $d < 0, k' < -1$ a two-sublattice model should be considered [18]. Let us note that in the region $d < 0, -0.1 > k' > -1$ in the vicinity of the line $k' = -1 - \frac{1}{3}d$ the regions with different numbers of various PTs exist. Construction of a projection of a phase diagram on (d, k') plane and study of thermodynamic properties of the model in these regions are subject of a separate paper.

In figures 2, 3 we show the phase diagrams in (t, d) plane for $k' = -0.1, 0.0, 1.0, 2.0, 2.6$ (regions II, III, IV), $k' = 2.88$ (regions II, III, VII, III, IV), $k' = 2.95$ (regions II, III, VII, I, IV), $k' = 3.2$ (regions II, III, VI, I, IV), $k' = 3.44$ (regions II, V, VI, I, IV), $k' = 4.0, 8.0, 20.0$ (regions II, V, I, IV). Hereafter our consideration will imply increasing temperature and decreasing single-ion anisotropy.

Let us briefly consider the pair CFs.

At the transition **FP2** (region II and V) the inverse CF G_{12}^{-1} has an infinite discontinuity ($G_{12}^{-1}(t_c - 0) = 0, G_{12}^{-1}(t_c + 0) = \infty$), whereas the inverse CF $G_{11}^{-1}(t_c) = 0$ (see figures 4, 5, 6, 9, 18, 22, 25). The inverse CF G_{22}^{-1} has a finite discontinuity ($G_{22}^{-1}(t_c - 0) < G_{22}^{-1}(t_c + 0)$), and always decreases in the phase **P**.

In the vicinity of the region $d > 0, k' < -1 - \frac{1}{6}d$ CFs $G_{11}^{-1}, G_{12}^{-1}, G_{22}^{-1}$ are finite and $q \neq 1, m \neq 1$ at $t = 0$ (see figures 4(c), 5(b)). A little bit away from the region $d > 0, k' < -1 - \frac{1}{6}d$ (increasing d or increasing k') the quantities $q, m, G_{11}^{-1}, G_{12}^{-1}, G_{22}^{-1}$ have bends at low temperature (see figure 4(b)). But a little bit farther from this region $d > 0, k' < -1 - \frac{1}{6}d$ this peculiarity in **F**-phase disappears.

Let us explore now the temperature behaviour of $G_{22}^{-1}(t > t_c)$ when k' increases and d decreases (approaching the region $d > 0, k' < -1 - \frac{1}{6}d$; the region III, the region V). Far from the regions III, V (see figures 4, 5, 6(a), 18(a)) $G_{22}^{-1}(t > t_c)$ decreases, and this decrease is not always related to a decrease in $q(t)$. For instance, at small negative k' in the vicinity of

Figure 1. The projection of the phase diagram onto $d - k'$ plane.

Figure 2. The phase diagram for the several values of k' is plotted in d and the reduced temperature plane. 1 - $k' = -0.1$; 2 - $k' = 0.0$; 3 - $k' = 1.0$; 4 - $k' = 2.0$; 5 - $k' = 2.6$; 6 - $k' = 2.88$; 7 - $k' = 2.95$; 8 - $k' = 3.2$; 9 - $k' = 3.44$; 10 - $k' = 4.0$.

Figure 3. The phase diagram for the several values of k' is plotted in d and the reduced temperature plane. 10 - $k' = 4.0$; 11 - $k' = 8.0$; 12 - $k' = 20.0$.

Figure 4. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q} = 0)$, $G_{22}^{-1}(\vec{q} = 0)$ at $k' = -4.0$ for different values of parameter d : (a) - $d = 30.0$; (b) - $d = 18.5$; (c) - $d = 18.0$.

Figure 5. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q} = 0)$, $G_{22}^{-1}(\vec{q} = 0)$ at $k' = -1.0$ for different values of parameter d : (a) – $d = 10.0$; (b) – $d = 0.0$

Figure 6. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q} = 0)$, $G_{22}^{-1}(\vec{q} = 0)$ at $k' = 0.0$ for different values of parameter d : (a) – $d = 5.0$; (b) – $d = -2.0$.

Figure 7. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q} = 0)$, $G_{22}^{-1}(\vec{q} = 0)$ at $k' = 0.0$ for different values of parameter d :
 (a) - $d = -2.825$; (b) - $d = -2.85$; (c) - $d = -2.95$;
 (d) - $d = -2.99$.

Figure 8. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q} = 0)$, $G_{22}^{-1}(\vec{q} = 0)$ at $k' = 1.0$ for different values of parameter d : (a) – $d = -5.725$; (b) – $d = -5.9$.

Figure 9. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q} = 0)$, $G_{22}^{-1}(\vec{q} = 0)$ at $k' = 2.0$ for different values of parameter d : (a) – $d = -4.0$; (b) – $d = -8.0$.

Figure 10. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q} = 0)$, $G_{22}^{-1}(\vec{q} = 0)$ at $k' = 2.0$ for different values of parameter d :
 (a) $-d = -8.5$; (b) $-d = -8.6$; (c) $-d = -8.7$;
 (d) $-d = -8.8$; (e) $-d = -8.9$; (f) $-d = -8.99$.
 (Parts (a), (b), (c), (d) of the figure are on previous page.)

the region $d > 0$, $k' < -1 - \frac{1}{6}d$ $q(t)$ increases, but $G_{22}^{-1}(t)$ decreases (see figure 5(b)). At small positive k' with decreasing d (approaching the region III) $G_{22}^{-1}(t > t_c)$ and $q(t > t_c)$ start to increase with temperature (see figure 6(b)), although at some values of parameters q decreases but G_{22}^{-1} increases (see figure 9(b)). At larger values of k' the decreasing of d (approaching the regions III, V and in the region V) lead to the fact that G_{22}^{-1} has a minimum in the **P**-phase (see figures 18(b), 22, 25).

At **FP1**, the inverse correlation function $G_{12}^{-1}(t)$ has an infinite discontinuity ($G_{12}^{-1}(t_c - 0) > 0$, $G_{12}^{-1}(t_c + 0) = \infty$), whereas CFs $G_{11}^{-1}(t)$ and $G_{22}^{-1}(t)$ have finite discontinuities and decrease in the **F**-phase. Let us analyse the behaviour of $G_{11}^{-1}(t)$ and $G_{22}^{-1}(t)$ in the vicinity of **FP1** phase transition and in the **P**-phase in the region III for $k' = 0.0, 1.0, 2.0, 2.6, 2.88, 2.95$ when the value of the single-ion anisotropy decreases (moving from the region II towards the region IV for $k' = 0.0, 1.0, 2.0, 2.6$; moving from the region II towards the region VII for $k' = 2.88, 2.95$; between the regions VII and IV for $k' = 2.88$), in regions III, VI for $k' = 3.2$ (moving from the region II towards the region I), and in region VI for $k' = 3.44$ (moving from the region V towards the region I). In the region III and near to the region II (see figures 7(a), 10(a), 11(a), 12(a), 15(a), 19) $G_{11}^{-1}(t_c - 0) > G_{11}^{-1}(t_c + 0)$, $G_{22}^{-1}(t_c - 0) < G_{22}^{-1}(t_c + 0)$, $G_{11}^{-1}(t > t_c)$ and $G_{22}^{-1}(t > t_c)$ increase at all considered values of k' except for $k' = 3.2$ (see figure 19), at which $G_{22}^{-1}(t)$ has a minimum in the **P**-phase. Let us consider the case $k' = 0$. When d decreases, minimums of $G_{11}^{-1}(t)$ (see figure 7(b)), and, then, of $G_{22}^{-1}(t)$

Figure 11. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q}=0)$, $G_{22}^{-1}(\vec{q}=0)$ at $k' = 2.6$ for different values of parameter d :
 (a) $-d = -10.4$; (b) $-d = -10.6$; (c) $-d = -10.625$;
 (d) $-d = -10.79$.

Figure 12. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q}=0)$, $G_{22}^{-1}(\vec{q}=0)$ at $k' = 2.88$ for different values of parameter d :
 (a) $-d = -11.5$; (b) $-d = -11.55$; (c) $-d = -11.59$;
 (d) $-d = -11.595$.

Figure 13. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q}=0)$, $G_{22}^{-1}(\vec{q}=0)$ at $k' = 2.88$ for $d = -11.61$.

Figure 14. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q}=0)$, $G_{22}^{-1}(\vec{q}=0)$ at $k' = 2.88$ for $d = -11.63$.

Figure 15. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q}=0)$, $G_{22}^{-1}(\vec{q}=0)$ at $k' = 2.95$ for different values of parameter d : (a) $-d = -11.7$; (b) $-d = -11.8$.

Figure 16. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q}=0)$, $G_{22}^{-1}(\vec{q}=0)$ at $k' = 2.95$ for different values of parameter d : (a) $-d = -11.84$; (b) $-d = -11.849$.

Figure 17. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q}=0)$, $G_{22}^{-1}(\vec{q}=0)$ at $k' = 2.95$ for $d = -11.86$.

(see figure 7(c)) appear in the paramagnetic phase. At smaller values of d $G_{22}^{-1}(t_c)$ decreases with a discontinuity (see figure 7(d)). For illustration, we depict in figure 8 the temperature dependences of G_{11}^{-1} , G_{22}^{-1} at $k' = 1.0$ (the changes in the temperature curves of single-site CFs and pair CFs with d are similar at $k' = 0$ and $k' = 1.0$) which correspond to two latter cases for $k' = 0$ (figures 7(c), 7(d)). At $k' = 2.0$ $G_{22}^{-1}(t_c)$ decreases with a discontinuity (see figure 10(b)) when d is decreased. Then, minima of $G_{11}^{-1}(t)$ (see figure 10(c)), and then, of $G_{22}^{-1}(t)$ (see figure 10(d)) appear in the **P**-phase. At smaller values of d at first $G_{11}^{-1}(t_c)$ has upward step (see figure 10(e)), but then again this step become downward (see figure 10(f)). That is, in the vicinity of the regions IV at $k'=0.0, 1.0, 2.0$ the behaviour

Figure 18. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q}=0)$, $G_{22}^{-1}(\vec{q}=0)$ at $k' = 3.2$ for different values of parameter d : (a) $-d = -5.0$; (b) $-d = -12.0$.

Figure 19. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q}=0)$, $G_{22}^{-1}(\vec{q}=0)$ at $k' = 3.2$ for $d = -12.47$.

Figure 20. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q}=0)$, $G_{22}^{-1}(\vec{q}=0)$ at $k' = 3.2$ for $d = -12.63$.

Figure 21. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q} = 0)$, $G_{22}^{-1}(\vec{q} = 0)$ at $k' = 3.2$ for different values of parameter d : (a) $-d = -12.673$; (b) $-d = -12.8$.

Figure 22. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q} = 0)$, $G_{22}^{-1}(\vec{q} = 0)$ at $k' = 3.44$ for $d = -13.34$.

of CFs $G_{11}^{-1}(t)$ and $G_{22}^{-1}(t)$ is qualitatively similar (see figures 7(d), 8(b), 10(f)). The changes in behaviour of CFs with decreasing of d at $k' = 2.6$ and $k' = 2.88$ are at first the same as those at $k' = 2.0$ (see figures 10(b), 11(b), 12(b), 10(c), 11(c), 12(c)). Near the region IV $G_{11}^{-1}(t_c)$ increases with a discontinuity at $k' = 2.6$ (see fig 11(d)). Behaviour of $G_{11}^{-1}(t)$ near the region VII at $k' = 2.88$ is similar to that at $k' = 2.6$ near the region IV, but CF $G_{22}^{-1}(t)$ has no minimum in the paramagnetic phase (see figures 11(d), 12(d)). Between the regions VII and IV a minimum of $G_{22}^{-1}(t > t_c)$ appears; the behaviour of $G_{11}^{-1}(t)$ and $G_{22}^{-1}(t)$ is the same as at $k' = 2.6$ near the region IV (see figures 11(d), 14)). At $k' = 2.95$ the region III is rather narrow, therefore, only $G_{22}^{-1}(t)$ behaviour is changes with a decrease in d

Figure 23. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q} = 0)$, $G_{22}^{-1}(\vec{q} = 0)$ at $k' = 3.44$ for different values of parameter d : (a) $-d = -13.42$; (b) $-d = -13.475$.

Figure 24. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q} = 0)$, $G_{22}^{-1}(\vec{q} = 0)$ at $k' = 3.44$ for different values of parameter d : (a) $-d = -13.48$; (b) $-d = -13.696$.

Figure 25. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q} = 0)$, $G_{22}^{-1}(\vec{q} = 0)$ at $k' = 4.0$ for different values of parameter d : (a) – $d = -15.1$; (b) – $d = -15.3$.

in this region (see figure 15(b)). Let us note that the changes in $G_{22}^{-1}(t)$ behaviour with d are the same as those at $k' = 2.0, 2.6, 2.88$ in the region III near the region II (see figures 10(b), 11(b), 12(b)). The behaviour of $G_{11}^{-1}(t)$ and $G_{22}^{-1}(t)$ at $k' = 3.2$ in the region VI (between the regions V and I) is qualitatively different from that at $k' = 0.0, 1.0, 2.0, 2.6, 2.88, 2.95$ near the region II (see figures 7(a), 10(a), 11(a), 12(a), 15(a)). Here $G_{22}^{-1}(t > t_c)$ (see figure 19) has a minimum (such behaviour of $G_{22}^{-1}(t)$ in the paramagnetic phase remains starting from the region II (see figure 18(b)). When the single-ion anisotropy is decreased (moving from the region II in regions III and VI) a minimum of $G_{22}^{-1}(t > t_c)$ disappears (see figure 20), and the behaviour of $G_{11}^{-1}(t)$ and $G_{22}^{-1}(t)$ becomes the same as at $k' = 0.0, 1.0, 2.0, 2.6, 2.88, 2.95$ near the region II (see figures 7(a), 10(a), 11(a), 12(a), 15(a)).

Let us consider now the behaviour of the inverse correlation functions $G_{11}^{-1}(t)$, $G_{12}^{-1}(t)$, $G_{22}^{-1}(t)$ at the phase transition **QP1** in regions I and VII (see figures 13, 16, 17, 21, 24, 26). Here, the inverse CF $G_{12}^{-1}(t)$ is infinitely large both in phases **Q** and **P**. The inverse CF $G_{11}^{-1}(t)$ has discontinuity, and $G_{11}^{-1}(t_c - 1) > G_{11}^{-1}(t_c + 0)$; $G_{11}^{-1}(t < t_c)$ decreases and $G_{11}^{-1}(t > t_c)$ can either increase or first decrease and then increase. The inverse CF $G_{22}^{-1}(t)$ has a cusp in the transition point. At $k' = 2.88$ in the entire region VII the inverse CF $G_{11}^{-1}(t)$ has a minimum in the paramagnetic phase (see figure 13). At $k' = 2.95, 3.2, 3.44, 4.0$, the $G_{11}^{-1}(t > t_c)$ increases (see figures 16(a), 21(a), 24(a), 26(a), 26(b)); a minimum of $G_{11}^{-1}(t > t_c)$ appears if d is decreased (see figures 16(b), 21(b), 24(b), 26(c)). Let us also note that almost always if $q(t)$ increases in the paramagnetic phase then $G_{11}^{-1}(t > t_c)$ has a minimum

Figure 26. The temperature dependences of m , q and CFs $G_{11}^{-1}(\vec{q} = 0)$, $G_{22}^{-1}(\vec{q} = 0)$ at $k' = 4.0$ for different values of parameter d : (a) - $d = -15.4$; (b) - $d = -15.6$; (c) - $d = -15.79$.

(see figures 13, 16(b), 17, 21(b), 24(b), 26(c)), and if $q(t > t_c)$ decreases then $G_{11}^{-1}(t > t_c)$ increases (see figures 21(a), 24(a), 26(a), 26(b)). However, it is possible that even if $q(t)$ increases in **P**, $G_{11}^{-1}(t > t_c)$ increases has no minimum (see figure 16(a)). The inverse CF $G_{22}^{-1}(t)$ increases in the paramagnetic phase at small k' (see figures 13, 16, 17, 21). At large values of k' in the close proximity to the region V, the $G_{22}^{-1}(t)$ decreases before the cusps at the transition point and after it and starts to increase only at higher temperatures (see figures 24, 26).

At the transition **FQ1** (region VII), the inverse CF $G_{12}^{-1}(t)$ has an infinite discontinuity ($G_{12}^{-1}(t_c - 0) > 0$, $G_{12}^{-1}(t_c + 0) = \infty$; $G_{12}^{-1}(t < t_c)$ decreases), whereas a discontinuity the inverse CFs $G_{11}^{-1}(t)$ and $G_{22}^{-1}(t)$ if finite. In phases **F**, **Q** inverse CFs $G_{11}^{-1}(t)$ and $G_{22}^{-1}(t)$ decrease, and $G_{11}^{-1}(t_c - 0) < G_{11}^{-1}(t_c + 0)$, $G_{22}^{-1}(t_c - 0) > G_{22}^{-1}(t_c + 0)$ (see fig 13, 16).

At the transition **QF1** (regions V, VI) the inverse CF $G_{12}^{-1}(t)$ has an infinite discontinuity ($G_{12}^{-1}(t_c - 0) = \infty$, $G_{12}^{-1}(t_c + 0) > 0$; $G_{12}^{-1}(t)$ decreases

in the phase **F**), whereas a discontinuity of $G_{11}^{-1}(t)$ and $G_{22}^{-1}(t)$ is finite, and $G_{11}^{-1}(t_c - 0) > G_{11}^{-1}(t_c + 0)$. In phases **Q** and **F**, inverse CFs $G_{11}^{-1}(t)$ and $G_{22}^{-1}(t)$ decreases (see figures 20, 22, 23, 25). At enough small values of k' and arbitrary d (see figure 20), and also at longer values of k' and enough large d (see figures 22, 23(a), 25(a)) $G_{22}^{-1}(t_c - 0) < G_{22}^{-1}(t_c + 0)$. At large k' and small d (see figures 23(b), 25(b)) $G_{22}^{-1}(t_c - 0) > G_{22}^{-1}(t_c + 0)$.

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НАБЛИЖЕННЯ ДВОЧАСТИНКОВОГО КЛАСТЕРА ДЛЯ ІЗІНГІВСЬКИХ МОДЕЛЕЙ З ДОВІЛЬНИМ ЗНАЧЕННЯМ СПІНА. КОРЕЛЯЦІЙНІ ФУНКЦІЇ МОДЕЛІ БЛЮМА-ЕМЕРІ-ГРІФІТСА

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В наближенні двочастинкового кластера досліджуються Ізінгівські моделі з довільним значенням спіна. Для цих моделей у випадку гіперкубічних ґраток отримано вирази для парних кореляційних функцій у $\vec{q}$ -просторі. У випадку простої кубічної ґратки для моделі Блюма-Емері-Гріфітса ($S = 1$) з білінійною K , біквадратичною K' взаємодіями та одноіонною анізотропією D побудована проекція фазової діаграми на площину $D/K - K'/K$. При різному наборі значень параметрів D/K та K'/K отримані температурні залежності $\langle S^z \rangle$, $\langle (S^z)^2 \rangle$ та парних кореляційних функцій при $\vec{q} = 0$.