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Tri-critical behavior of the Blume Capel model on a diamond lattice

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ABSTRACT

The mean field approximation results are obtained in a five-site cluster on the diamond lattice from the Bogoliubov inequality. Spin correlation identities for the Blume-Capel model on diamond lattice are derived from a five-site cluster and used to obtain an effective field approximation. The free-energy, magnetization, critical frontiers and tricritical points are obtained from the mean field approximation and the effective field approximation and are compared to those obtained by other methods. From the mean-field approximation, we also studied the unstable and metastable states besides the stable states present in the model.

1. Introduction

The Blume-Capel model (BC) was introduced by Blume [1] and independently by Capel [2]. This model can be applied to describe many different physical situations such as multicomponent fluids, ternary alloys, ^{3}He^{4}He mixtures and various magnetic problems [3]. The Hamiltonian of the Blume-Capel model is given by

$$H = -\sum_{i,j} J_{ij} S_i S_j + D \sum_i S_i^2, \tag{1}$$

where $J_{ij} > 0$, D is the single ion anisotropy and the first sum is over the nearest neighbors spins on the lattice. Each S_i is restricted by $S_i = \{-1, 0, +1\}$.

The Blume-Capel model on rectangular and hexagonal lattices exhibits a variety of multicritical phenomena such as a phase diagram with ordered ferromagnetic (F) and disordered paramagnetic (P) phases separated by a transition line that changes from a continuous phase transition to a first-order phase transition at a tricritical point (T_t). This model is also a generalization of the standard Ising model. In the limit of $D \to \infty$ one recovers the two-state Ising model with $S_i = \pm 1$. By increasing the value of D, we have a decrease of T_c. Moreover, at zero temperature, the first-order transition line ends at the point $D_c/J = z/2$, where z is the coordination number of the lattice [4,5].

The spin-1 Blume-Capel model was studied by a variety of methods such as mean-field approximation (MFA) [1,2], effective-field approximation (EFA) [4–11], the Bethe lattice approximation [12], series expansion method (SE) [13,14], cluster variation method (CVM) [15,16], Monte Carlo (MC) simulations [17–20], renormalization-group (RG) method [21,22] and rigorous inequality correlation function [23–25]. Most of these studies were done on hexagonal and rectangular lattices.

The MFA [1,2] was the first technique used to obtain an approximate solution to the Blume-Capel model. The EFA is one of the first improvements over the MFA. The EFA was used by Honmura and Kaneyoshi [26] to study the spin-1/2 Ising model and has been generalized to treat the spin-1 model [7]. This conventional EFA includes spin-spin correlations resulting from the usage of the van der Waerden relation and provides results that are superior to those obtained within the traditional MFA. The critical behavior of the Blume Emery Griffiths (BEG) spin 1 model on a diamond lattice (see Fig. 1) was studied within the framework of a finite cluster theory [28]. In this study it was used an expansion technique for the cluster identities that allows the kinematic properties of the spin operators be accounted for in a systematic way. Ekiz et al. [15,29] studied the unstable and metastable phases present in the BC and BEG models..

The aim of the present work is to study the spin-1 Blume-Capel model on the diamond lattice in a cluster of spins with five sites (see Fig. 2), to obtain the multicritical phenomena. The five-site cluster contains all the symmetries of the diamond lattice. To accomplish this objective, we present a generalization of the mean field approximation for the model of spin-1 Blume-Capel in a five-site cluster on the diamond lattice, using the Bogoliubov inequality [30–32], getting results for free-energy, phase diagrams and magnetization. To study the EFA, we derive a correlation function identity for a cluster of spins with five sites. From the correlation identities we obtain results for the magnetization, phase transitions lines and tricritical points with the

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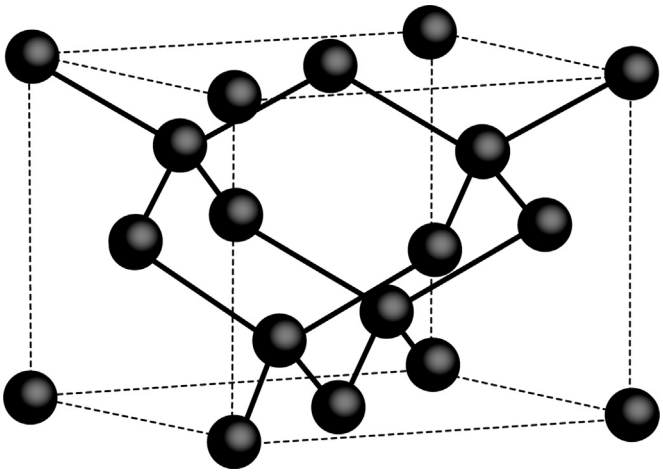

Fig. 1. Diamond lattice.

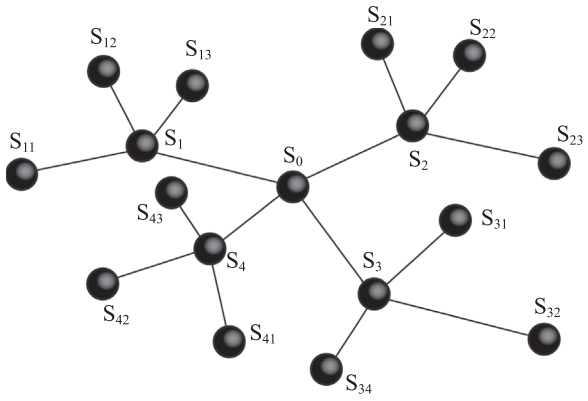

Fig. 2. Structure of five-site cluster for the diamond lattice.

application of the EFA which, as has been said previously, includes the effects of autocorrelations through the usage of the van der Waerden identities and provide results that are superior to those obtained within the MFA. In the application of the EFA a free-energy functional [4–6] was used to obtain the line of first order transitions. We remark that the results obtained improve over the one-site MFA and the one-site EFA because the five-site cluster contains more correlations than the one-site cluster. Moreover, the one-site MFA and EFA give the results for the two dimensional square lattice, which definitely are the wrong results for the diamond lattice. From the mean-field approximation, we also studied the unstable and metastable states besides the stable states present in the model..

The Section 2 is devoted to the mean field approximation, to obtain expressions for free energy and magnetization, in a five-site cluster of the spin-1 Blume-Capel model on the diamond lattice starting from the Bogoliubov inequality. In Section 3.1, we present the derivation of the correlation identities for the five-site cluster of the spin-1 Blume-Capel model on the diamond lattice, which are an extension of Callen's identity for spin 1/2 Ising model [33] and for the spin-1 Blume-Capel model for the one-site cluster [7]. The correlation identity for the spin-1 Blume-Capel model obtained from the one-site cluster is suitable to study the model in hexagonal and rectangular lattices. However, for the diamond lattice this one-site correlation identity does not contain the symmetries of the lattice. In this case one has to rely on clusters which contain all the symmetries of the lattice, which is the case of the five-site cluster, shown in Fig. 2. In Section 3.2, from these identities, derived in the previous section, we obtain the EFA and apply them to get the phase diagrams. The correlation identities can be used to derive rigorous upper bounds on critical temperatures using inequalities for the higher order correlation functions. However, this will not be done here. In Section 4, we present the numerical results and the phase diagrams as compared to other methods and in Section 5, we make the concluding remarks.

2. Mean field approximations

In this section we use the mean field approximation for Blume-Capel model on the diamond lattice starting from the Bogoliubov inequality [30–32], to obtain results for free-energy, phase diagrams and magnetization. The mean-field theory presumes a virtual independence of the spins variables, which is achieved by the renormalization of the actual magnetic field to the effective field taking into account the contribution from the averaged nearest-neighbor interactions. The foremost advantage of the mean-field theory lies in that it can be readily generalized to more complex lattice-statistical models as for instance the spin-1 Blume-Capel model [1,2], which may even display a greater versatility of the critical behavior including a change of continuous phase transitions to discontinuous ones at a tricritical point.

The Hamiltonian of the Blume-Capel model, is given by

$$H = -J \sum_{\langle i,j \rangle}^{Nz/2} S_i S_j + D \sum_{i=1}^{N} S_i^2, \tag{2}$$

where N denotes the total number of the lattice sites and z is their coordination number.

The Bogoliubov variational principle is based on a validity of the inequality [30–32]:

$$G \leq \phi = G_0 + \langle H - H_0 \rangle_0, \tag{3}$$

where G and H represent the true Gibbs free energy and the full Hamiltonian of a considered lattice-statistical model, whereas G_0 and H_0 represent the trial Gibbs free energy and the trial Hamiltonian of a simplified lattice-statistical model for which the relevant calculations can be performed exactly (the symbol $\langle \ldots \rangle_0$ denotes canonical ensemble average within the simplified model defined by the Hamiltonian H_0). The expression ϕ represents the variational Gibbs free energy, which provides an upper bound for the true Gibbs free energy G.

Here we present a generalization of the mean field theory for the model of spin-1 Blume-Capel in a five-site cluster on the diamond lattice, using the Bogoliubov inequality. The objective of developing the mean field theory on a higher of cluster ($n > 1$) is to maintain the symmetry of the lattice. For example the square, Kagome and diamond lattices exhibit the same coordination number (z=4) and different symmetries. To accomplish this we use within the mean-field approximation a summation over the frontier sites of a cluster of five sites of the diamond lattice (see Fig. 2) and replaces an expectation value for all other spins by the mean value. Hence, it follows that the Hamiltonian of five spin is at the mean-field level, given by

$$H_5 = -\left(JS_0 \sum_{j=1}^{4} S_j + J \sum_{j=1}^{4} S_j \left(\sum_{k=1}^{3} \langle S_{jk} \rangle \right) - DS_0^2 - D \sum_{j=1}^{4} S_j^2 \right). \tag{4}$$

H_5 is the Hamiltonian describing the site 0 and its neighbors j = 1, 2, 3, 4 and S_{jk} are the neighbors of sites j.

According to this, the mean-field approximation of the spin-1 Blume-Capel in a five-site cluster on the diamond lattice (see Fig. 2) can be accomplished by the following choice of the trial Hamiltonian,

$$H_0 = -\sum_{\langle j,0 \rangle}^{N'} \left(JS_0 \sum_{j=1}^{4} S_j + \sum_{j=1}^{4} \gamma_j S_j - DS_0^2 - \sum_{j=1}^{4} \eta_j S_j^2 \right), \tag{5}$$

which depends on two different variational parameters γ_j and η_j with the physical meaning of an effective field. The N' denotes the total number of the cluster with five sites on the diamond lattice ($N' = N/5$).

Eq. (5) has the physical meaning of the effective field and the effective single-ion anisotropy acting on a spin and quadrupolar