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Phase Diagram for Spin-1 Blume Capel Model with a Special Random Crystal Field

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The spin-1 Blume-Capel model with a special random crystal field was studied in the Pair Approximation based on Bogoliubov inequality for the free energy. The global phase diagram in the reduced temperature as a function of reduced anisotropy plane for the whole range of concentration was obtained. Special interest is given in the low temperature region of the phase diagrams where a number of first-order lines emerge from a multiphase point at the ground state. The results for the two- and three-dimensional models are qualitatively the same and, as the two-dimensional model is more studied in the literature, we will just discuss below the phase diagrams for the square lattice z = 4. A lower critical concentration (p⋆), above which there is no more a stable ferromagnetic phase at low temperatures for arbitrarily large values of the crystal field, is achieved from the present approach. There are three different intervals for the probability concentration of crystal field. The first interval is $p_1^\star < p < 1$ where $p_1^\star$ is approximated to 0.93, the phase diagram presents a tricritical point, two different ordered phases at low temperatures, and is similar to that of the pure model. The second interval is $p^\star < p < p_1^\star$ with $p^\star = (z-2)\,/\,(z-1)$, where the reentrance and the tricritical point are disappeared. And finally, for p < p⋆ where there is an asymmetric second-order transition line extending infinitely for d $\rightarrow \infty$ and two distinct ferromagnetic phases at low temperatures separated by a first-order transition line ending at an isolated multiphase critical point.

Keywords: Blume Capel model;random crystal field;phase diagram;pair approximation.

A trav´es de la aproximación de pares basada en la desigualdad de Bogoliubov se estudió el modelo de Blume-Capel con un campo cristalino aleatorio especial. Se obtuvó un diagrama de fases global en el plano de la temperatura reducida como función de la anisotropia reducidad para todo el rango de concentración. La región que llamó la atención es aquella a bajas temperaturas donde un número de líneas de primer orden emergen desde un punto multifásico en el estado fundamental. Los resultados para un modelo en dos y tres dimensiones son cualitativamente los mismos y, como el modelo bidimensional es el más estudiado, se discutirá los diagramas de fases para una red cuadrada z = 4. Se obtuvo con la presente aproximación una concentración crítica mínima (p⋆), por encima de la cual no hay más una fase ferromagnética estable a bajas temperaturas para valores muy grandes del campo cristalino. Hay tres intervalos diferentes para la probabilidad de concentración del campo cristalino. El primer intervalo es $p_1^\star < p < 1$ donde $p_1^\star$ es aproximadamente 0.93, los diagramas de fases presentan un punto tricrítico, dos fases ordenadas a bajas temperaturas y es muy similar al modelo puro (p = 1). El segundo es $p^\star < p < p_1^\star$ con $p^\star = (z-2)\,/\,(z-1)$, donde las reentrancias y el punto tricrítico desaparecen. Y, finalmenten, p < p⋆ donde hay una línea de transición de segundo orden asimétrica que se extiende para d $\rightarrow \infty$ y dos fases feromagnéticas diferentes a bajas temperaturas separadas por una línea de transición de primer orden que finaliza en un punto crítico multifásico.

Descriptores: Modelo de Blume Capel;campo cristalino aleatorio;diagrama de fases; aproximación de pares.

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1. Introduction

The Blume Capel model has been extensively studied since its introduction nearly 40 years ago. This model was proposed to describe magnetic materials with single ion anisotropy [1,2]. Its Hamiltonian is given by:

$$H = J\sum_{(ij)}\sigma_i\sigma_j + \sum_i \Delta_i\sigma_i^2 \qquad (1)$$

where the first sum runs over all pairs of nearest neighbors in the N lattice sites, σ_i is the spin-1 Ising operator and there are three possible states for each site: spin up (3/4 = 1), spin down (σ = -1), or vacant (σ = 0), J is the spin-spin interaction between nearest neighbors and Δ_i is the single-ion anisotropy or an energy to favor or penalize vacancies.

For J > 0 (ferromagnetic case) this model exhibits critical behavior such as first- or second-order transitions and one TriCritical Point (TCP). Recently, some interest has been directed to the understanding of systems in the presence of random crystal fields. It has been shown that this system has a very rich multicritical behavior and many interesting phenomena can appear, i.e., the reentrance behavior or the existence of isolated critical points [3,4].

The pure model for values of spin $\sigma > 1$ has been treated by mean field [5], pair approximation and Monte Carlo simulations in three-dimensions, [6], and more recently by means of conventional finite-size scaling, conformal invariance and Monte Carlo simulations in two-dimensions [7]. It has been shown that for integer spins there exist one tricritical point and a paramagnetic phase at low temperatures which are not present for semiinteger spins. In both cases, there are a number of firstorder lines emerging from a multiphase point at T = 0 and Δ/zJ = 0.5 inside the ferromagnetic region.

For integer spins one has σ lines where $\sigma - 1$ of them end up at independent isolated multiphase critical points while the other one joins the second-order transition line at the tricritical point. For semi-integer spins all the $\sigma - 1/2$ lines terminate at independent isolated multiphase critical points.

The Blume-Capel random model is treated by choosing the probability distribution function P(Δ_i), given by

$$P\left(\Delta_i\right) = p\delta\left(\Delta_i - \Delta\right) + \left(1-p\right)\delta\left(\Delta_i + \Delta\right) \qquad (2)$$

In this paper the Blume-Capel random is studied by the pair approximation based on Bogoliubov inequality for the free energy [8], and the global phase diagram is obtained through the numerical analysis of the minimum of its free-energy.

The outline of the present paper is as follows: In Sec. 2 we develop the pair approximation for the model taking special probability distribution function. The results are presented in Sec. 3 for σ = 1 and some concluding remarks are given in Sec. 4.

2. Pair approximation

2.1. Materials

The problem can be treated following Ref. 3. The one-site (H_s) and two-site (H_p) Hamiltonians are:

$$H_s = \gamma_s\sigma_1 - \delta_s\sigma_1^2 + \Delta\sigma_1^2 \qquad (3)$$

$$H_p = -J\sigma_1\sigma_2 - \gamma_p\left(\sigma_1+\sigma_2\right) - \delta_p\left(\sigma_1^2+\sigma_2^2\right) + \Delta\left(\sigma_1^2+\sigma_2^2\right) \qquad (4)$$

where $\gamma_s, \delta_s, \gamma_p$ and δ_p are variational parameters to be found by minimizing the free energy

$$F \equiv \left(1-z\right)F_s + \frac{z}{2}F_p + \left(1-z\right)\left(\gamma_s m + \delta_s q\right) + z\left(\gamma_p m + \delta_p q\right) \qquad (5)$$

where z is coordination number of the lattice and the mean values $m \equiv \left(\left(\sigma_i\right)\right)_i$ and $p \equiv \left(\left(\sigma_i^2\right)\right)_i$ can be obtained from the one- and two-spin Hamiltonians:

$$m = \frac{\partial F_s}{\partial\left(\beta\gamma_s\right)} = \frac{1}{2}\frac{\partial F_p}{\partial\left(\beta\gamma_p\right)} \qquad (6)$$

and

$$q = \frac{\partial F_s}{\partial\left(\beta\delta_s\right)} = \frac{1}{2}\frac{\partial F_p}{\partial\left(\beta\delta_p\right)} \qquad (7)$$

Minimization of Eq. (5) with respect to the variational parameters leads to

$$\left(z-1\right)\gamma_s = z\gamma_p, \left(z-1\right)\delta_s = z\delta_p(7) \qquad (8)$$

Thermodynamic properties are obtained from Eqs. (5-7), but some features of the phase diagram can be determined analytically. For instance, close to the secondorder phase transition one has $m\simeq 0$ and also $\gamma_s\simeq 0$ and $\gamma_p\simeq 0$, so (5) can be expanded in powers of m (Landau like expansion)

$$F = F_0 + \frac{1}{2}a_2\left(T,\Delta\right)m^2 + \frac{1}{4}a_4\left(T,\Delta\right)m^4 + \frac{1}{6}a_6 m^6(8) \qquad (9)$$

The second-order line is given by $a_2\left(T,\Delta\right) = 0$ with $a_4 > 0$ and the TCP is located at $a_2\left(T,\Delta\right)=0$, $a_4\left(T,\Delta\right)=0$ with $a_6 > 0$.

3. Results and discussions

Blume-Capel random on a square lattice (z = 4) was analyzed within the PA and the numerical analysis showed three different behavior, as a function of the concentration of Δ, of the global phase diagram by solving Eqs. (6b). The results are depicted in Figs. 1-3, where $t = kBT/J$ and .

For $p_1^\star < p < 1$ with $p_1^\star\simeq 0.93$, there is a TCP and two different ordered phases (O1 with magnetization m1 = 1 and O2 with m2 = 1 − p are illustrated in Fig. 1) at low temperatures. The pronounced reentrance transition line at low temperature could be an artifact of the present method, once the PA sometimes gives incorrect results for systems in which there is a competition in ordering [9], but other approximation used by other authors have been showed similar bahavior [4,10,11]. Second- and first-order transition lines linked by the TCP.

For $p^\star < p < p_1^\star$ with $p_1^\star = (z-2)/(z-1)$, the reentrance and the TCP are disappeared. Instead, the corresponding second-order transition line ends at a critical end point, the first-order line separating the ferromagnetic phase from the paramagnetic one ends at an isolated multiphase critical point immersed in the ferromagnetic phase (see Fig. 2).

Finally, the Fig. 3 illustrates the last behavior for $p < p^\star$ where there is an asymmetric second-order transition line ex-

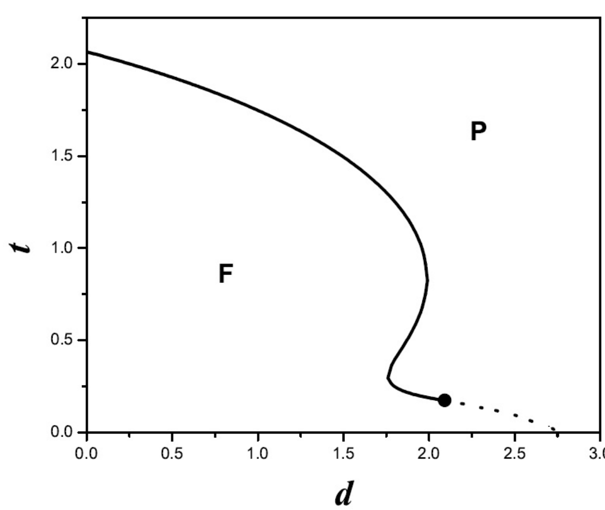

FIGURE 1. Phase diagram in the d − t plane of the two-dimensional random crystal field model for p = 0.97. Solid and dashed lines represent the second- and first-order transitions. Dark circle indicates tricritical point.

tending infinitely for d $\rightarrow \infty$ and two distinct ferromagnetic phases at low temperatures separated by a first-order transition line ending at an isolated multiphase critical point.

4. Concluding remarks

The spin σ = 1 Blume-Capel model with special random crystal field has been studied by means of the pair approximation. A variety of rich phase diagrams has been achieved, some of them new and different from those predicted through mean field approximation and effective field theory. We have for the two-dimensional model:

1. For $p_1^\star < p < 1$, with $p_1^\star \simeq 0.93$, the system presents a tricritical point and two different ordered phases at low temperatures;

2. For $p^\star < p < p_1^\star$, where $p_1^\star = (z-2)/(z-1)$ the phase diagrams are similar. However, we have no tricritical points. Instead, the corresponding second-order transition line ends at a critical end point and the first-order line penetrates into the ferromagnetic phase terminating in an isolated critical point.

3. Finally, for $p < p^\star$, the second-order transition line extends to the infinity as $\Delta \rightarrow \infty$.

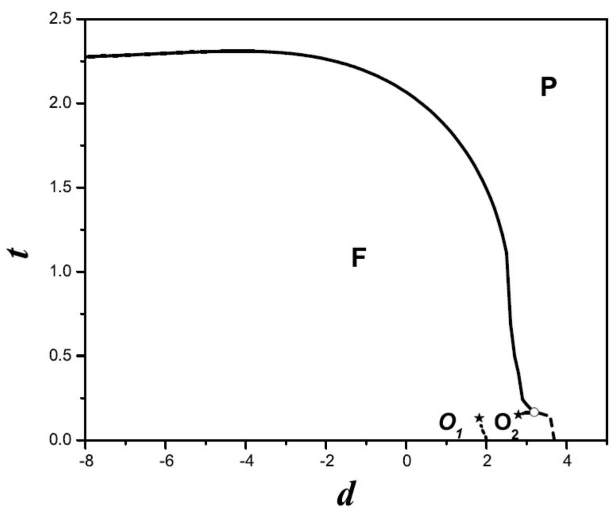

FIGURE 2. The same as Fig. 1 for p = 0.8. White circle and asterisk are critical end and isolated multiphase critical points, respectively. O1 and O2 are two ordered phases.

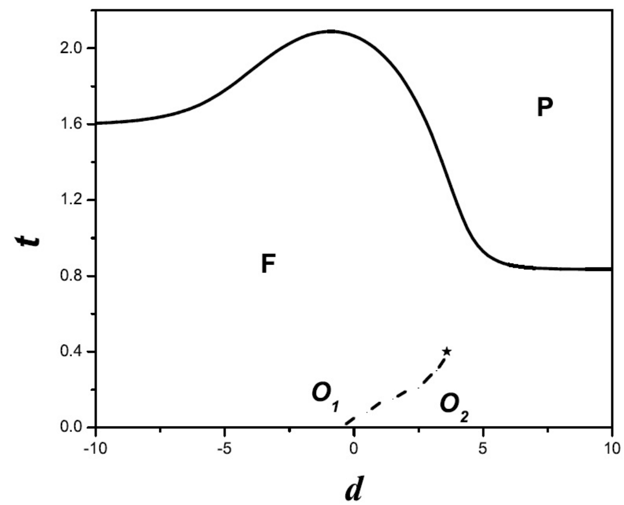

FIGURE 3. The same as Fig. 1 for p = 0.6, where O1 and O2 correspond to magnetizations m1 = 1 and m2 = 1 − p, respectively.

Just the phase diagrams in the iii) case above are analogous to those from mean field approximation. Although the existence of a $p^\star$ is in agreement with more reliable results of effective field theory, the latter approach is not capable to determine the complex structure of the ferromagnetic phases at low temperatures. This same qualitative behavior is also found for the three-dimensional version of the model.

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