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Mean-field study of the degenerate Blume–Emery–Griffiths model in a random crystal field[1]

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Abstract

The degenerate Blume–Emery–Griffiths (DBEG) model has recently been introduced in the study of martensitic transformation problems. This model has the same Hamiltonian as the standard Blume–Emery–Griffiths (BEG) model but, to take into account vibrational effects on the martensitic transition, it is assumed that the states $S=0$ have a degeneracy p ($p=1$ corresponds to the usual BEG model). This model was studied by E. Vives et al. for a particular value of Δ, through a mean-field approximation and numerical simulation. When the parameter p increases, the ferromagnetic phase shrinks and the region where the transition is of first order increases. In some materials, however, the transition would be better described by a disordered DBEG model; further, the inclusion of disorder in the DBEG model may be relevant in the study of shape memory alloys. From the theoretical point of view, it would be interesting to study the consequence of conflicting effects: the parameter p, which increases the first-order phase-transition region, and disorder in the crystal field, which tends to diminish this region in three dimensions. In order to study this competition in high-dimensional systems, we apply a mean-field approximation: it is then possible to determine the critical behavior of the random DBEG model for any value of the interaction parameters. Finally, we comment on (preliminary) results obtained for a two-dimensional system, where the randomness in the crystal field has a more drastic effect, when compared to the three-dimensional model.

Keywords: Multicritical phase diagrams; Disordered models; Mean-field approximation

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1. Introduction

The Blume–Emery–Griffiths (BEG) model has been invented a long time ago, in the context of fluid mixtures [1]. The Hamiltonian of the model reads

$$\mathscr{H} = -J \sum_{\langle i,j \rangle} S_i S_j - K \sum_{\langle i,j \rangle} S_i^2 S_j^2 + \Delta \sum_i S_i^2 \,, \tag{1}$$

where J is the exchange constant, K is the biquadratic interaction, Δ is a crystal field, the first two sums are over nearest-neighbor pairs on a lattice, the third sum is over all sites and $S_i = \pm 1, 0$. Its phase diagram presents first order and continuous transitions, as well as multicritical points. More recently, a generalization of the BEG model was introduced, the so-called degenerate Blume–Emery–Griffiths (DBEG) model [2]. Its hamiltonian is given by Eq. (1) but the $S = 0$ states have a degeneracy p ($p = 1$ is equivalent to the BEG model). This parameter mimics the effects of vibrational degrees of freedom on the martensitic transitions. The DBEG model was studied, for a particular value of the crystal field, within a mean-field approximation and Monte-Carlo simulation: the effect of p is to shrink the ferromagnetic phase and to increase the region where the transition is of first order [2].

Nevertheless, some materials were found to be better described by a disordered DBEG model, which may be relevant in the description of conventional shape memory alloys as well [2]. From the theoretical point of view, on the other hand, it has been shown that randomness may have drastic consequences on multicritical behavior. In two dimensions, for instance, any infinitesimal amount of disorder suppresses non-symmetry-breaking first-order phase transitions and replaces symmetry-breaking first-order phase transitions by continuous ones. The effect of disorder on high-dimensional systems is different: first-order phase transitions disappear only at a finite amount of randomness [3,4]. This behavior has been observed in a large variety of models, either with "field" or with "interaction" randomness [3–6].

So, in the disordered DBEG model two ingredients have opposite effects: while the degeneracy factor p increases the region where the transition is of first order, disorder tends to suppress this region. This competition may have interesting effects on the phase diagrams, apart from potential experimental relevance. In order to study these effects on high-dimensional systems, we apply a mean-field approximation to the DBEG model on a random crystal field. The disordered parameter is the crystal field, which follows a probabilistic distribution:

$$\mathscr{P}(\Delta_i) = r\delta(\Delta_i + \Delta) + (1 - r)\delta(\Delta_i - \Delta) \,. \tag{2}$$

In fact, the exact form of this distribution does not affect the qualitative results; we comment later where quantitative aspects depend on the probability distribution. It is worth stressing that, if the interaction parameters, J and K, were chosen to be random, instead of the crystal field, the overall consequences on the phase diagram would be the same [3,4].

2. Formalism and results

Our approximation is based on the Gibbs inequality for the free energy [7]:

$$F \leqslant \mathrm{Tr}\rho\,\mathscr{H} + (1/\beta)\mathrm{Tr}\rho\ln\rho\,, \tag{3}$$

where F is the exact free energy, $\mathscr{H}$ is the DBEG Hamiltonian and ρ is an exactly solvable density matrix. We chose ρ as the most general single-site density matrix for the ferromagnetic (positive J and K) system.

The right-hand side of the previous equation is then minimized with respect to the variational parameters. The configurational averages, taken with respect to the random fields, are then made on the resulting equations. We then obtain equations in the form

$$f = \int \mathscr{P}(\Delta_i)\mathscr{F}(J,K,\Delta_i,p;m,q)\,d\Delta_i\,, \tag{4}$$

$$m = \int \mathscr{P}(\Delta_i)\mathscr{M}(J,K,\Delta_i,p;m,q)\,d\Delta_i\,, \tag{5}$$

$$q = \int \mathscr{P}(\Delta_i)\mathscr{Q}(J,K,\Delta_i,p;m,q)\,d\Delta_i\,, \tag{6}$$

where $\mathscr{P}(\Delta_i)$ is given by Eq. (2), $m=[\langle S_i\rangle]_c$, $q=[\langle S_i^2\rangle]_c$ ($\langle\cdots\rangle$ and $[\cdots]$ are the thermal and configurational averages, respectively) and $\mathscr{M}$, $\mathscr{Q}$ and $\mathscr{F}$ are the expressions for m, q and the free energy, respectively, for an arbitrary distribution of crystal fields. In general, one obtains more than one solution to these equations. The solution which minimizes Eq. (4) is the equilibrium state. Since this procedure is usual, we will not discuss it in detail.

Let us first comment on some general results we obtain, for any K/J. The transition at zero temperature is not affected by the parameter p and takes place at $(\Delta/zJ)=(K/J+1)(1+r)/2$; for smaller values of Δ/zJ the magnetization equals 1, while $m=r$ for $\Delta/zJ>(K/J+1)(1+r)/2$.

For $\Delta/zJ=\infty$, the random field DBEG model, with the field distribution given by Eq. (2), is equivalent to the quenched site-diluted spin-$\frac{1}{2}$ Ising model. The states $S=\pm1$ represent magnetic sites and the states $S=0$ represent non-magnetic impurities. Therefore, only for $r\geqslant r_c$ (where r_c is the lattice-dependent value of r where an infinite cluster of present sites is formed for the first time, when r is increased from zero) the critical line between O and D (see figures) should extend to $\Delta/J=\infty$. For $r<r_c$, the "tail" of continuous transition would touch the zero-temperature axis at a finite value of Δ/zJ. The reason we find this "tail" extending to $\Delta/J=\infty$ for any $r\neq0$ is that the present approximation is equivalent to a model with infinite-range interactions (see Ref. [5]).

The asymptotic value of kT/zJ for $\Delta/zJ=\infty$ equals r; it does not depend on K and p. This result comes from the mapping between the *spin-*$\frac{1}{2}$ site-diluted Ising model and the limit $\Delta/zJ=\infty$, *which holds when the probability distribution is given by Eq.* (2). In this case, the degeneracy of the $S=0$ states and the biquadratic interaction

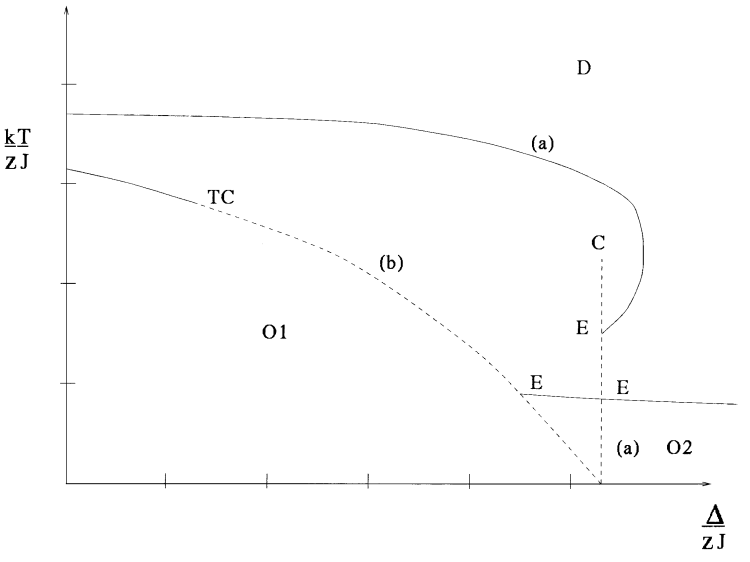

Fig. 1. Phase diagram of the random-field DBEG model, for $K/J = 0$ and $r = 0.1$. Dashed (continuous) lines indicate first-order (continuous) transition, k is the Boltzman constant, T is the temperature and z is the coordination number of the lattice. $O1(O2)$ stands for the ordered phase with $m = 1$ $(m = r)$ at $T = 0$, D stands for the disordered phase, C stands for critical points, E stands for critical end points, and TC stands for tricritical points. Finally, (a) stands for $p = 1$, while (b) stands for $p = 3$. The diagram for $r = 0$ is qualitatively the same as the curve (b), except for the $O2$ phase, which is no longer present.

K play no role in the dynamics of the $S = \pm 1$ states. If the distribution $\mathscr{P}(\Delta_i) = r\delta(\Delta_i) + (1 - r)\delta(\Delta_i - \Delta)$ is used, a different result will hold. The limit $\Delta/zJ = \infty$ is now equivalent to the *spin*-1 site-diluted Ising model; therefore, K and p are relevant and the asymptotic value of kT/zJ depends on both parameters.

The value of the kT/zJ (z is the coordination number of the lattice) for the tricritical points does not depend on p. This is an artifact of the mean-field approximation; results obtained using a real-space renormalization-group procedure on a two-dimensional lattice show a different behavior [8]. For the random model ($r \neq 0$), the temperature of tricritical points, critical end points and critical points shows a very weak dependence on p for $K/J = 5$, while the dependence is stronger for $K/J = 0$. In fact, the only effect of the degeneracy parameter in the phase diagram, for high values of K/J, is to shrink the ferromagnetic phase. Therefore, we aptly depict only the phase diagrams for $K/J = 0$, where qualitative changes occur when p is varied.

In Figs. 1 and 2 we show the $kT/zJ \times \Delta/zJ$ phase diagram for $K/J = 0$ and for some values of p. Note that qualitative changes occur when p is increased. For $r = 0.1$, the reentrant behavior observed for $p = 1$ is lost and a tricritical point is introduced for $p = 3$. This latter curve is qualitatively equivalent to the phase diagram for r close to zero. For $r = 0.3$ a reentrant behavior is obtained for high enough p (curve (c)); a critical end point (E), which was not present for $p = 1$ and $p = 3$ is also observed.

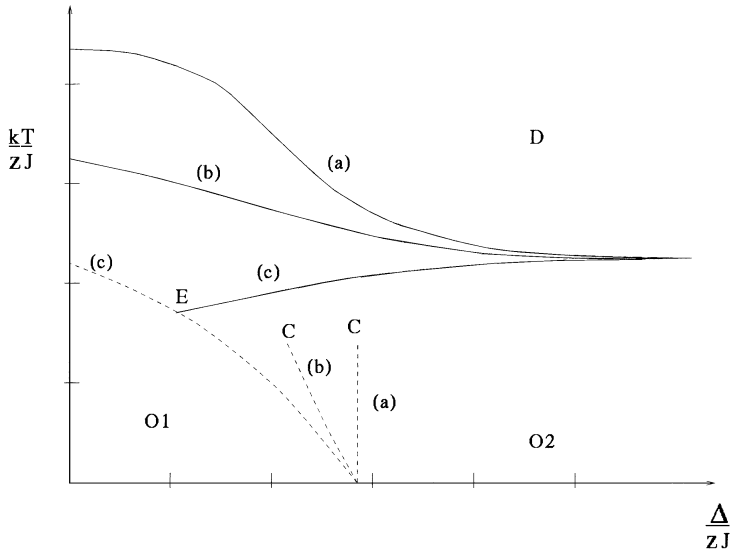

Fig. 2. Phase diagram of the random-field DBEG model, for $K/J = 0$ and $r = 0.3$. Same notation as in Fig. 1; (c) stands for $p = 7$. Note the qualitative change for $p > 3$: a critical end point is present for $p = 7$, as well as reentrant behavior, with order–disorder–order transitions as Δ/zJ is increased from small values.

The first-order transition curve for $p = 7$ extends to negative values of Δ/zJ, until it reaches a line of continuous transitions at a tricritical point [not depicted in Fig. 2].

3. Conclusion

Using a mean-field approximation, we calculate the phase diagrams for the random crystal field DBEG model, varying the degree of disorder, r, and the degeneracy factor, p. For high values of K/J the phase diagrams are almost insensitive to the value of p, while for $K/J = 0$ the dependence on p is stronger. Moreover, for the latter value of K/J and $r = 0.3$ the phase diagram changes qualitatively when p is increased enough: while for $p = 1$, for instance, the order–disorder transition is always continuous and the first-order transition inside the ordered phase ends in a critical point, for $p = 7$ a line of first-order transition separates the ordered and disordered phases at low values of Δ/zJ. A reentrant behavior is obtained for high p. For $K = 0$ and $r = 0.1$, the degeneracy reintroduces a tricritical point and eliminates the reentrant behavior.

Some of the features found in this work may be an artifact of the simple mean-field approximation we used and should not hold for a low-dimensional system. Preliminary results for the square lattice, using a real-space renormalization-group approach, show a different behavior: for any infinitesimal amount of disorder the first-order transition is suppressed, independent of p [8].

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