Reentrant phase transitions in the Blume-Emery-Griffiths model on a simple cubic lattice: The two-particle cluster approximation

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The two-particle cluster approximation is applied to study the reentrant and double reentrant behaviors of the spin-1 Ising model with nearest-neighbor bilinear and biquadratic exchange interactions and single-ion anisotropy on a simple cubic lattice. The phase diagrams are constructed and the temperature dependences of dipolar and quadrupolar moments are calculated at various values of model parameters (at those when it suffices to consider a one-sublattice problem).

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I. INTRODUCTION

The Blume-Emery-Griffiths model (BEG) corresponding to a spin-1 Ising system is one of the most extensively studied models in condensed-matter physics. That is so not only because of the relative simplicity with which approximate calculations for this model can be carried out and tested, as well as of the fundamental theoretical interest arising from the richness of the phase diagram that is exhibited due to the competition of interactions, but also because versions and extensions of the model can be applied for the description of simple and multicomponent fluids,[1–3] dipolar and quadrupolar orderings in magnets,[3–5] crystals with ferromagnetic impurities,[3] ordering in semiconducting alloys,[6] etc.

The BEG Hamiltonian is given by

$$H=-\sum_{i=1}^{N} DS_i^2-\frac{1}{2}\sum_{i,\delta}\left[KS_iS_{i+\delta}+K'S_i^2S_{i+\delta}^2\right], \qquad (1)$$

where $S_i=0,\pm 1$, D is a single-ion anisotropy energy, K and K' are the constants of bilinear and biquadratic short-range interaction, and the summation i,δ is going over nearest-neighbor pairs.

The BEG model has been investigated by different techniques: using the mean-field approximation (MFA),[1–4,7] effective-field theory,[8–11] two-particle cluster approximation (TPCA),[12–14] Bethe approximation,[15] high-temperature series expansions,[16] renormalization-group theory (RG),[17,18] and Monte Carlo simulations.[15,19–21] At certain sets of the model parameters, the BEG model on three-dimensional lattices can undergo several kinds of reentrant and double reentrant phase transitions (PT) against temperature (see Refs. 7, 15, and 21).

It should be noted that at zero single-ion anisotropy, the TPCA (results of which coincide with results of the constant-coupling and Bethe approximations), unlike the MFA, correctly responds to the competition between ferromagnetic bilinear and antiferromagnetic biquadratic interactions. The phase diagrams obtained within TPCA for different lattice types[12,15] qualitatively agree with the Monte Carlo simulations results.[19,21] We would like to mention that the phase diagrams presented in Refs. 12 and 21 in the temperature vs biquadratic interaction plane at zero single-ion anisotropy are not complete (the line separating the quadrupole and staggered quadrupole phases is absent, since only the one-sublattice model was considered).

In this paper we study the BEG model on a simple cubic lattice within TPCA at such values of antiferromagnetic biquadratic interaction and a single-ion anisotropy (bilinear interaction is ferromagnetic: $K>0$), when reentrant and double reentrant phase transitions between the quadrupole phase and the ferromagnetic phase take place. We restrict our consideration to those values of the parameters ($K'/K>-1$) at which it suffices to consider a one-sublattice problem. This problem has been approached within Bethe approximation,[15] MFA,[7] and within renormalization-group theory.[18] However, Ref. 15 contains certain errors in numerical calculations; therefore, the phase diagrams presented there and some of the conclusions drawn are qualitatively incorrect.

II. THE TWO-PARTICLE CLUSTER APPROXIMATION

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

$$H_1=-\tilde{\varkappa}S_1-\tilde{\varkappa}'S_1^2, \quad \tilde{\varkappa}=\Gamma+z\varphi, \quad \tilde{\varkappa}'=D+z\varphi', \qquad (2)$$

(z is the number of nearest neighbors, magnetic field $\Gamma\to 0$ is introduced for convenience) and a two-particle Hamiltonian H_{12},

$$H_{12}=-\tilde{\tilde{\varkappa}}(S_1+S_2)-\tilde{\tilde{\varkappa}}'(S_1^2+S_2^2)-KS_1S_2-K'S_1^2S_2^2, \qquad (3)$$

$$\tilde{\tilde{\varkappa}}=\Gamma+(z-1)\varphi, \quad \tilde{\tilde{\varkappa}}'=D+(z-1)\varphi'$$

in a usual way.[12,13,22]

$$F=-k_BTN\left[(1-z)\ln Z_1+\frac{z}{2}\ln Z_{12}\right], \qquad (4)$$

$$Z_1=2e^{\beta\tilde{\varkappa}'}\cosh(\beta\tilde{\varkappa})+1, \qquad (5)$$

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

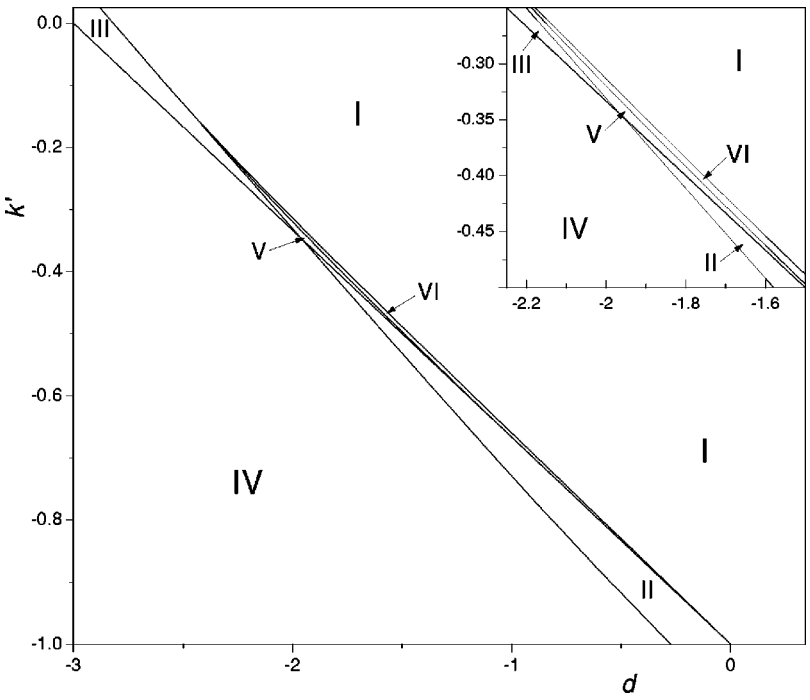

FIG. 1. The projection of the phase diagram onto the $(d,\ k')$ plane.

Here $\beta=(k_{\mathrm{B}}T)^{-1}$. The cluster parameters φ and φ' are found by minimizing the free energy with respect to them. The following system of equations for φ and φ' is obtained:

$$\frac{e^{\beta\tilde{\varkappa}'}\sinh(\beta\tilde{\varkappa})}{Z_1} = \frac{\exp[\beta(2\tilde{\tilde{\varkappa}}'+K'+K)]\sinh(2\beta\tilde{\tilde{\varkappa}})+e^{\beta\tilde{\tilde{\varkappa}}'}\sinh(\beta\tilde{\tilde{\varkappa}})}{Z_{12}}, \tag{6}$$

$$\frac{e^{\beta\tilde{\varkappa}'}\cosh(\beta\tilde{\varkappa})}{Z_1} = \frac{e^{\beta(2\tilde{\tilde{\varkappa}}'+K')}[e^{\beta K}\cosh(2\beta\tilde{\tilde{\varkappa}})+e^{-\beta K}]+e^{\beta\tilde{\tilde{\varkappa}}'}\cosh(\beta\tilde{\tilde{\varkappa}})}{Z_{12}}.$$

Using Eqs. (6) we can write simple expressions for magnetization $m=\langle S\rangle$ and quadrupolar moment $q=\langle S^2\rangle$,

$$m=\frac{2e^{\beta\tilde{\varkappa}'}\sinh(\beta\tilde{\varkappa})}{Z_1}, \quad q=\frac{2e^{\beta\tilde{\varkappa}'}\cosh(\beta\tilde{\varkappa})}{Z_1}. \tag{7}$$

Hereafter we shall use the terminology of Ref. 15: F, the ferromagnetic phase $(m\neq 0,\ q\neq\frac{2}{3})$; Q, the quadrupolar phase $(m=0,\ q\neq\frac{2}{3})$; SQ, the staggered quadrupole phase (two-sublattice ordering; m of the both sublattices are zero, whereas the quadrupolar moments of the sublattices are different). We also introduce the notations $k'=K'/K$, $d=D/K$, and $t=k_{\mathrm{B}}T/(zK)$.

It should be remembered[7,15,17–19] that the equations presented above (with a single q and single m for the whole lattice) cannot be used in the entire space of the model parameters, since at certain sets of k', d, t the SQ ordering takes place (with different q for different sublattices). Thus, for a simple cubic lattice this happens[15] at the sets of the parameters from the regions $k'<-1$ and $d_1<d<-6k'-6$ (d_1 depends on k': $d_1=0,-0.6,-1.2$ for $k'=-1,\ -2.25,\ -3.85$, respectively). The line $d=-6k'-6$ at $k'<-1$ separates the F and SQ orderings in the ground state (d,k') phase diagram.[15] This accords with the (k',t) phase diagrams obtained within Bethe approximation[15] at those values of the model parameters when the transitions $Q\rightarrow F\rightarrow Q\rightarrow SQ$, $Q\rightarrow F\rightarrow SQ$, $Q\rightarrow SQ$ take place upon lowering temperature. The values $d_1=0,-0.6,-1.2$ (and the corresponding $k'=-1,\ -2.25,\ -3.85$) are found from the (k',t) phase diagrams[15] at different values of d as the points where the reentrant PT's, $Q\rightarrow SQ\rightarrow Q$, emerge (Bethe approximation result).

Let us consider results of our numerical calculations. The projection of the phase diagram obtained within the TPCA of

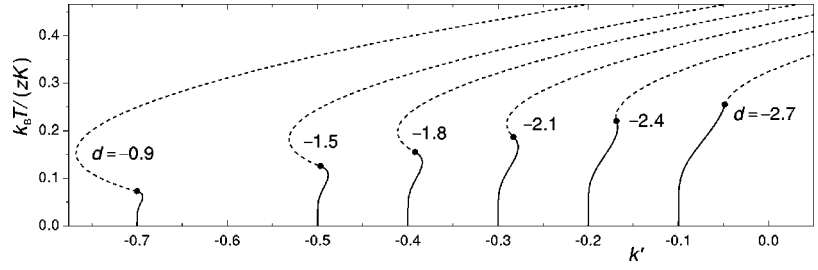

FIG. 2. The k' vs reduced temperature phase diagrams for several values of d. The dashed and solid lines represents the second-order and first-order phase transitions, respectively. The circles denote the tricritical points.

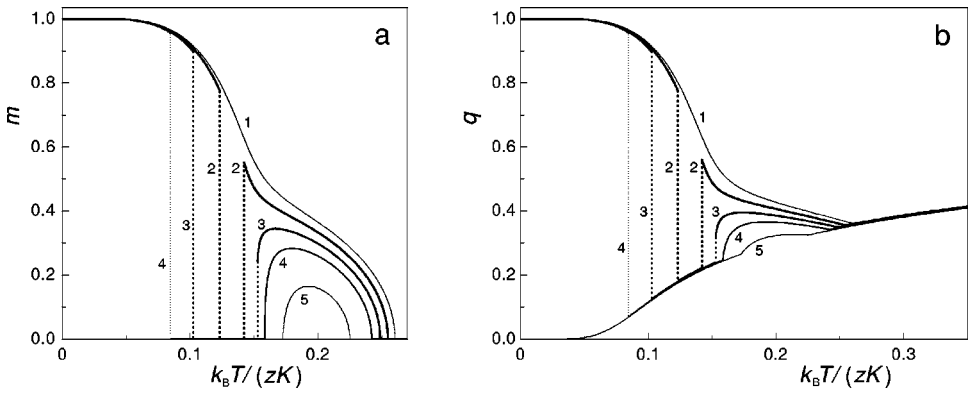

FIG. 3. The temperature dependences of m (a) and q (b) at $d=-1.8$ for different values of parameter k': (1) $k'=-0.38$; (2) $k'=-0.385$; (3) $k'=-0.39$; (4) $k'=-0.395$; (5) $k'=-0.405$.

the BEG model on a simple cubic lattice on the (d, k') plane at $-1<k'\leqslant 0$ (see Fig. 1) consists of six regions: *I*, the $Q \rightarrow F$ phase transition of the second order (which takes place in the system upon lowering temperature); II, the reentrant $Q\rightarrow F\rightarrow Q$ PT's, both being of the second order; III, the $Q \rightarrow F$ PT of the first order; IV, the PT is absent; V, the double reentrant $Q\rightarrow F\rightarrow Q\rightarrow F$ PT's and only the lower transition is of the first order; VI, the double reentrant $Q\rightarrow F\rightarrow Q \rightarrow F$ PT's and only the upper transition is of the second order. Let us note that the regions III and IV, as well as the regions V and II are separated by the line $k'=-1-d/3$ (the same line that separates the perfect zero ordering and ferromagnetic ordering regions in the ground state[15]).

The phase diagrams in the k' vs reduced temperature plane for several values of d are shown in Fig. 2. One can see the general aspect of the phase transitions against the temperature considered in the model at $-1<k'\leqslant 0$ (within TPCA). Let us consider, for instance, the case of $d=-1.8$ (see also Fig. 3). At $k'>-0.384$ there is only one second-order PT $Q\rightarrow F$ in the system. At $k'\in\,]-0.4,-0.384]$ there are double reentrant PT's, $Q\rightarrow F\rightarrow Q\rightarrow F$, and at $k'\in [-0.392,-0.384]$ only the upper transition is of the second order, while at $k'\in\,]-0.4,-0.392[$ only the lower PT is of the first order. $k'=-0.392$, $t=0.155$ are tricritical point coordinates (k'_{TCP}, t_{TCP}, where the line of the second-order phase transitions meets a line of the first-order phase transitions). At $k'\in[-0.411,-0.4]$ there are reentrant PT's, $Q \rightarrow F\rightarrow Q$, in the system, both being of the second order.

The analogous (k',t) phase diagrams presented in Ref. 15 obtained within the Bethe approximation are qualitatively different from ours in the vicinity of the tricritical points. At the tricritical point, the line of the phase transitions obtained in Ref. 15 has a cusp, while both second-order and first-order parts of the phase boundary come to the tricritical point from the left [at $k'=k'_{\mathrm{TCP}}+0$ only one second-order PT, $Q\rightarrow F$ occurs in the system]. The authors of Ref. 15 concluded that at those sets of model parameters, when the double reentrant PT's, $Q\rightarrow F\rightarrow Q\rightarrow F$, against the temperature took place in the system, only the lower PT could be of the first order. Since the self-consistent equations obtained in Ref. 15 within the Bethe approximation in a single-sublattice case coincide with relations (6) and (7) obtained within TPCA, an error in numerical calculations performed in Ref. 15 must have been made.

Let us briefly compare the results obtained above with the results of other methods. First of all, at $-1<k'<0$, the changes in the topology of the (d,t) phase diagrams with k' are similar (as can be readily seen in Fig. 1) to the changes in the topology of the (k',t) diagrams with d (Fig. 2). Within the TPCA at $-1<k'<k'_{\mathrm{R,TPCA}}$ ($k'_{\mathrm{R,TPCA}}\approx -0.16$), the (d,t) phase diagrams are of a double reentrant topology with a tricritical point [Fig. 4(c)]. In contrast, within the MFA,[7] the (d,t) phase diagrams are of a double reentrant topology with a tricritical point only at $-0.18<k'<k'_{\mathrm{R,MFA}}$ ($k'_{\mathrm{R,MFA}}<0$, the value of $k'_{\mathrm{R,MFA}}$ is not given in Ref. 7). Within both the TPCA and MFA, the middle PT can be either of the first or of the second order. At $-1<k'<-0.18$, the phase diagrams within the MFA are of a topology [Fig. 4(a)] that is not predicted by the TPCA: the second-order phase transition line terminates at the critical end point *E* at the first-order PT line, the latter terminating at the critical point *C* inside the ferromagnetic phase.[7] This result is somewhat similar to that of the renormalization-group theory.[18] In the (d,t) phase dia-

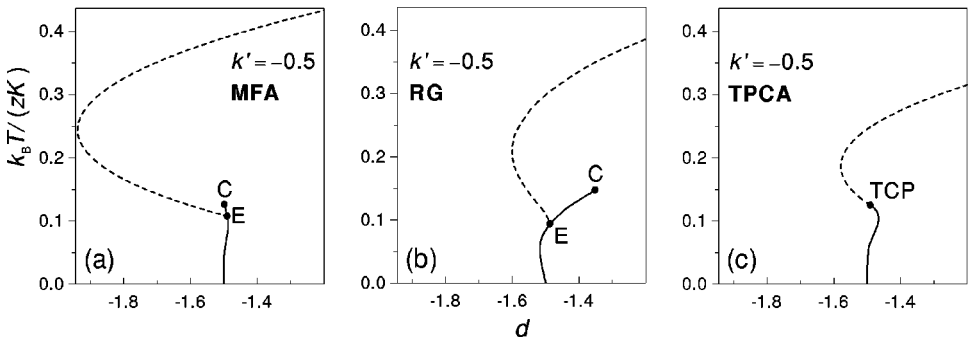

FIG. 4. The d vs reduced temperature phase diagrams for $k'=-0.5$ within MFA (Ref. 7) (a), renormalization-group theory (Ref. 18) (b), and TPCA (c). The dashed and solid lines represents the second-order and first-order phase transitions, respectively. The circles denote the critical end point *E*, critical point *C* (inside the ferromagnetic phase), and tricritical point (TCP).

gram obtained in Ref. 18 at $k'=-0.5$ [see Fig. 4(b)], the line of the second-order phase transitions also terminates at the critical end point E on the line of the first-order PT's, which, in its turn, terminates at the critical point C inside the ferromagnetic phase. However, the topologies of the first-order PT lines obtained with the MFA and RG methods[18] are qualitatively different [Fig. 4(a,b)]. Thus, within the MFA the part of this line corresponding to the $F\rightarrow Q$ transitions (with decreasing temperature) lies above the part corresponding to the $Q\rightarrow F$ PT's. In contrast, with the RG method[18] the $F\rightarrow Q$ part lies below the $Q\rightarrow F$ part. The critical point C lies to the left from the critical end point E within the MFA and to the right within the RG method. That is, at $k'=-0.5$ and fixed d at which the system undergoes the first-order PT's, the MFA and RG methods[18] predict qualitatively different cascades of the PT's with changing temperature.

At $k'=-1$, the (d,t) phase diagrams obtained within the RG method,[18] MFA,[7] and within the TPCA are of a single reentrant topology (see Fig. 5). At $d=0$, the temperature of the second-order PT, $Q\rightarrow F$, obtained within the TPCA is much closer to the corresponding temperature calculated by Monte Carlo simulations[21] than those found within the RG method[18] or MFA.[7]

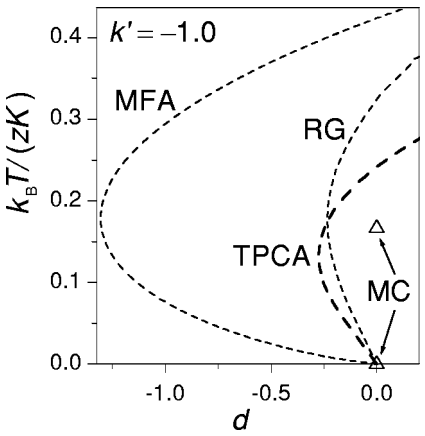

FIG. 5. The d vs reduced temperature phase diagrams for $k'=-1.0$ within MFA (Ref. 7), renormalization-group theory (Ref. 18) and TPCA. The dashed line represents the second-order phase transitions. The triangles denote the phase-transition temperatures at $k'=-1.0$, $d=0$ within Monte Carlo simulations (Ref. 21).

III. CONCLUSIONS

The phase diagrams of the Blume-Emery-Griffiths model on a simple cubic lattice have been constructed at those sets of model parameters for which the double reentrant phase transitions $Q\rightarrow F\rightarrow Q\rightarrow F$ against the temperature occur in the system. It was shown that within TPCA the middle PT can be of the first and of the second order [similarly as within the MFA (Ref. 7) at those sets of the model parameters when analogous phase transitions occur]. Let us recall that Ref. 15 (Bethe approximation) contains errors in numerical calculations. As a result, an incorrect conclusion has been drawn that at those sets of the parameters when the $Q\rightarrow F\rightarrow Q\rightarrow F$ phase transitions take place in the system, only the lower PT can be of the first order. We also show that the (d,k',t) phase diagram at $0>k'>-1$ obtained within the TPCA, MFA,[7] and renormalization-group theory[18] are qualitatively different.

[1] D. Mukamel and M. Blume, Phys. Rev. A **10**, 610 (1974).
[2] D. Furman, S. Dattagupta, and R.B. Griffiths, Phys. Rev. B **15**, 441 (1977).
[3] J. Sivardiere, in *Proceedings of the International Conference on Static Critical Phenomena in Inhomogeneous Systems, Karpacz*, 1984, Lecture Notes in Physics, Vol. 206 (Springer-Verlag, Berlin, 1984).
[4] H.H. Chen and P.M. Levy, Phys. Rev. B **7**, 4267 (1973).
[5] E.L. Nagaev, *Magnetics with Complicated Exchange Interaction*, (Nauka, Moscow, 1988).
[6] K.E. Newman and J.D. Dow, Phys. Rev. B **27**, 7495 (1983).
[7] W. Hoston and A.N. Berker, Phys. Rev. Lett. **67**, 1027 (1991).
[8] T. Kaneyoshi and E.F. Sarmento, Physica A **152**, 343 (1988).
[9] J.W. Tucker, J. Magn. Magn. Mater. **87**, 16 (1990).
[10] K.G. Chakraborty, Phys. Rev. B **29**, 1454 (1984).
[11] A.F. Siqueira and I.P. Fittipaldi, Phys. Status Solidi B **119**, K31 (1983).
[12] S.I. Sorokov, R.R. Levitskii, and O.R. Baran, Ukr. Fiz. Zh. **41**, 490 (1996) (in Ukrainian).
[13] S.I. Sorokov, R.R. Levitskii, and O.R. Baran, Condens. Matter Phys. **9**, 57 (1997).
[14] O.R. Baran and R.R. Levitskii, Phys. Status Solidi B **219**, 357 (2000).
[15] K. Kasono and I. Ono, Z. Phys. B: Condens. Matter **88**, 205 (1992).
[16] D. Saul, M. Wortis, and D. Stauffer, Phys. Rev. B **9**, 4964 (1974).
[17] A. Bakchick, A. Benyoussef, and M. Touzani, Physica A **186**, 524 (1992).
[18] R.R. Netz and A.N. Berker, Phys. Rev. B **47**, 15 019 (1993).
[19] R.J.C. Booth, Lu Hua, J.W. Tucker, C.M. Care, and I. Halliday, J. Magn. Magn. Mater. **128**, 117 (1993).
[20] D. Peňa Lara and J.A. Plascak, Int. J. Mod. Phys. B **12**, 2045 (1998).
[21] O.F. De Alcantara Bonfim and C.H. Obcemea, Z. Phys. B: Condens. Matter **64**, 469 (1986).
[22] J.S. Smart, *Effective Field Theories of Magnetism* (Saunders, Philadelphia, 1996).