Phase diagrams of the spin-1 Blume-Capel film with an alternating crystal field

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The spin-1 ferromagnetic Blume-Capel film with an alternating crystal field $\Delta=\Delta_1$ on the odd layers and $\Delta=\Delta_2$ on the even ones is considered in the mean-field approximation. The ground-state phase diagrams in the (d_1,d_2) plane ($d_1=\Delta_1/J$ and $d_2=\Delta_2/J$) are determined analytically; the number of their phases depends on the parity of the number of layers of the film. At finite temperature, 15 types of topology, depending on the range of variation of d_1, are found in the (t,d_2) plane for an even number of layers, but only 14 for an odd number of layers ($t=k_BT/J$ is the reduced temperature). The phase diagrams exhibit a variety of multicritical points. In particular, a tricritical point C appears in the paramagnetic-ferromagnetic line of transition, but only for values of d_1 larger than a threshold value $d_{trc}^{(2)}$ which is but the tricritical crystal field (in the mean-field approximation) of the spin-1 Blume-Capel model on a square lattice. Moreover, lines of transition presenting the reentrant and double reentrant behaviors may also take place.

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I. INTRODUCTION

The Blume-Capel (BC) model is a spin-1 Ising model with single-ion anisotropy. It has been originally introduced to study first-order magnetic phase transitions[1,2] and then applied to multicomponent fluids.[3] Later, it was generalized to the Blume-Emery-Griffiths model[4] to study the He^3-He^4 mixtures and a variety of other physical systems.

The BC model has been investigated in detail using many approximate methods, namely, mean-field approximation,[1,2] high temperature series expansion,[5] constant-coupling approximation,[6] Monte-Carlo[7] and renormalization-group[8] techniques. All of these approximate schemes suggest the existence of a tricritical point at which the system changes from the second-order phase transition to the first-order one, when the transition temperature is plotted as a function of the parameter of anisotropy.

On the other hand the BC model has been investigated on semiinfinite lattices with modified surface coupling. Several approximate methods have been used[9] (and references therein). All of them show the possibility to have a phase with ordered surface and disordered bulk, and show the existence of the so-called "extraordinary," "surface" and "ordinary" transitions, and of multicritical points called special points.[10] More recently, with the development of the molecular beam epitaxy technique and its application to the growth of thin metallic films, renewed interest in thin film magnetism has been stimulated, and much experimental and theoretical efforts have been devoted to the subject.[11] The BC model with a rationally decreasing crystal field has recently been extended to a layered structure and analyzed in the mean-field approximation.[12] The model exhibits a constant tricritical point and a reentrant phenomenon for a certain number of layers.

Our aim in this work is to study, using mean-field theory, the phase diagrams of a ferromagnetic spin-1 Blume-Capel film with an alternating crystal field: $\Delta=\Delta_1$ on the odd layers and $\Delta=\Delta_2$ on the even ones. The number of topologies of the phase diagrams is finite and depends only on the parity of the number of layers of the film. The phase diagrams present many multicritical points and may have transition lines exhibiting the reentrant and double-reentrant behaviors; this kind of behavior has been previously found in the Paramagnetic-Ferromagnetic transition line of the ordinary Blume-Capel model with a random crystal field[13] or with random nearest-neighbor interactions.[14]

The paper is organized as follows. In Sec. II we present the model and give the mean-field equations of the different order parameters. In Sec. III we present the results, then we end in Sec. IV by a conclusion.

II. MODEL AND METHOD

The system we consider is the spin-1 Blume-Capel model of a simple-cubic lattice, infinite and symmetric in the x and y directions and of finite thickness in the z direction, i.e., a film of N ferromagnetically coupled layers with an alternating crystal field. The Hamiltonian of this system is given by

$$\mathcal{H}=-J\sum_{\langle i,j\rangle} S_iS_j+\sum_i \Delta_i S_i^2, \tag{1}$$

where $S_i=\pm 1,0$; the first sum runs over all pairs of nearest neighbors and Δ_i is the crystal field which takes the value Δ_1 on the odd layers and Δ_2 on the even ones. The mean-field equations of state are straightforwardly obtained and are given by

$$m_k=\langle S_k\rangle=\frac{2\sinh\beta h_k}{e^{\beta\Delta_k}+2\cosh\beta h_k}, \tag{2}$$

$$q_k=\langle S_k^2\rangle=\frac{2\cosh\beta h_k}{e^{\beta\Delta_k}+2\cosh\beta h_k}, \tag{3}$$

with

$$h_1 = J(zm_1 + m_2),$$

$$h_k = J(m_{k-1} + zm_k + m_{k+1}) \quad \text{for} \quad 2 \leqslant k \leqslant N-1, \quad (4)$$

$$h_N = J(m_{N-1} + zm_N).$$

In these equations, m_k (q_k) is the reduced magnetization (quadrupolar moment) of the kth layer; and z is the interlayer coordination number ($z=4$ for the case of the square layers considered here). The reduced total magnetization is $m = (1/N)\Sigma_{k=1}^{N} m_k$. The reduced free energy of the film is given by

$$f = -\frac{1}{\beta}\sum_{k=1}^{N} \ln[1 + 2e^{-\beta\Delta_k}\cosh\beta h_k] + \frac{1}{2}\sum_{k=2}^{N-1}(m_{k-1} + zm_k + m_{k+1})m_k + \frac{1}{2}m_1(4m_1 + m_2) + \frac{1}{2}m_N(m_{N-1} + 4m_N). \quad (5)$$

III. RESULTS AND DISCUSSIONS

The study of the phase diagrams in the (t,d_2) plane exhibits the existence of different topologies depending on the range of variation of d_1 ($d_1 = \Delta_1/J$, $d_2 = \Delta_2/J$, and $t = k_B T/J$ are the values of the reduced crystal fields and temperature respectively). We note from the beginning that these topologies are limited in number and do not depend on the number of layers itself but only on its parity. In the following we will discuss in detail the case of an even number of layers and comment at the end on the odd number case. To understand the origin of the different topologies, we first determine analytically the ground-state phase diagram in the (d_1,d_2) plane by looking for the lowest-energy configurations. For an arbitrary even number of layers $N=2L$, we distinguish six regions of this plane [Fig. 1(a)] (but only five for an odd number of layers [Fig. 1(b))]. (a) $d_1<3$, $d_2<3$, and $d_1+d_2<6-1/L$; the stable configuration (see Ref. 16) for the notations) is $(11)^L$, where the spins of the sites of all the layers are all equal to 1. (b) $3<d_1<4$, $d_2<d_1$ and $(L-1)d_1+Ld_2<6L-4$; the stable configuration is $01(11)^{L-1}$, where the spins of the first layer are all equal to 0 while those of the other layers are all equal to 1. (c) $d_1>4$ and $d_2<2$; the stable configuration is $(01)^L$ where the spins of the odd layers are all equal to 0 while those of the even ones are all equal to 1. (d) $3<d_2<4$, $d_1<d_2$, and $Ld_1+(L-1)d_2<6L-4$; the stable configuration is $(11)^{L-1}10$. (e) $d_1<2$ and $d_2>4$; the stable configuration is $(10)^L$. (f) $d_1>2$, $d_2>2$, $d_1+d_2>6-1/L$, $(L-1)d_1+Ld_2>6L-4$ and $Ld_1+(L-1)d_2>6L-4$; the stable configuration is the nonmagnetic state $(00)^L$.

From Fig. 1(a) it is clear that for fixed values of d_1, the system exhibits various transitions by varying d_2. For the following ranges of variation of d_1: (i) $0<d_1<2$, (ii) $2<d_1<3-1/L$, (iii) $3-1/L<d_1<3$, (iv) $3<d_1<4$, and (v) $d_1>4$, the system presents the following phase transitions.

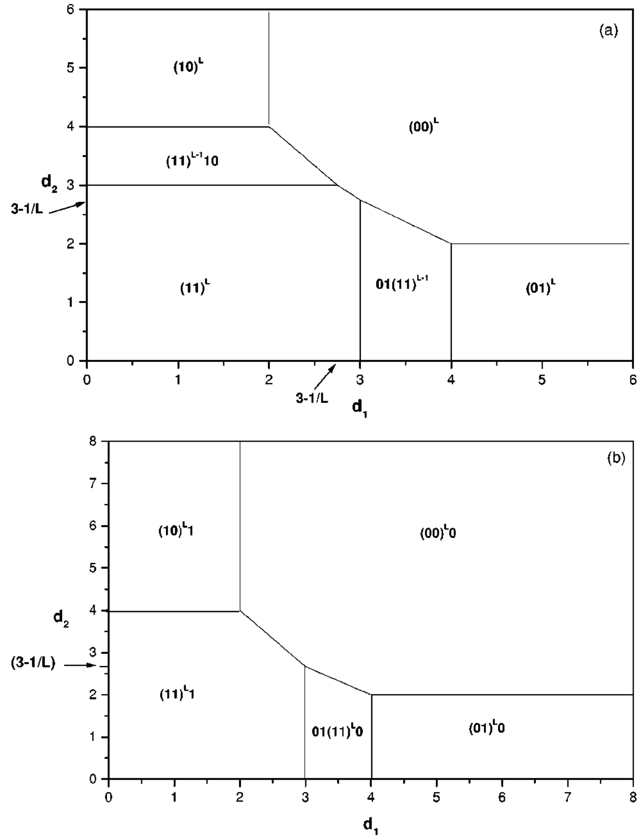

FIG. 1. The ground-state phase diagrams in the (d_1,d_2) plane for an arbitrary number N of layers, (a) $N=2L$, (b) $N=2L+1$.

(i) From the state $(11)^L$ to the state $(11)^{L-1}10$ at $d_2=3$ and then to the state $(00)^L$ at $d_2=4$. (ii) From the state $(11)^L$ to the state $(11)^{L-1}10$ at $d_2=3$ and then to the state $(00)^L$ at $Ld_2=(6L-4)-(L-1)d_1$. (iii) From the state $(11)^L$ to the state $(00)^L$ at $d_2=(6-1/L)-d_1$. (iv) From the state $01(11)^{L-1}$ to the state $(00)^L$ at $(L-1)d_2=(6L-4)-Ld_1$. (v) From the state $(01)^L$ to the state $(00)^L$ at $d_2=2$, respectively.

It is worth to note here that, contrary to the two- or three-dimensional Blume-Capel cases (or the case of a film with a homogenous crystal field), the ground-state of certain layers may be magnetic even for relatively large values of the crystal field in these layers. For example, for $d_1<2$, the even layers (except the final one) are in the magnetic states $m_{2k}=1$ even with a crystal field, in these layers, reaching the value $d_2=4$ [which is larger than the critical crystal field for a square ($d_c^{(2)}=2$) or three dimensional cubic ($d_c^{(3)}=3$) lattices].

For finite temperatures the transition lines are determined by solving numerically Eq. (2) which may have more than one solution; the one which minimizes the free energy [Eq. (5)] corresponds to the stable phase. Transitions of the second order are characterized by a continuous vanishing of the magnetizations while those of the first order exhibit discontinuities at the transition points.

In order to describe the different entities in the phase diagrams, the Griffiths notations[15] will be adopted: the critical end-point B^mA^n denotes the intersection of m lines of second

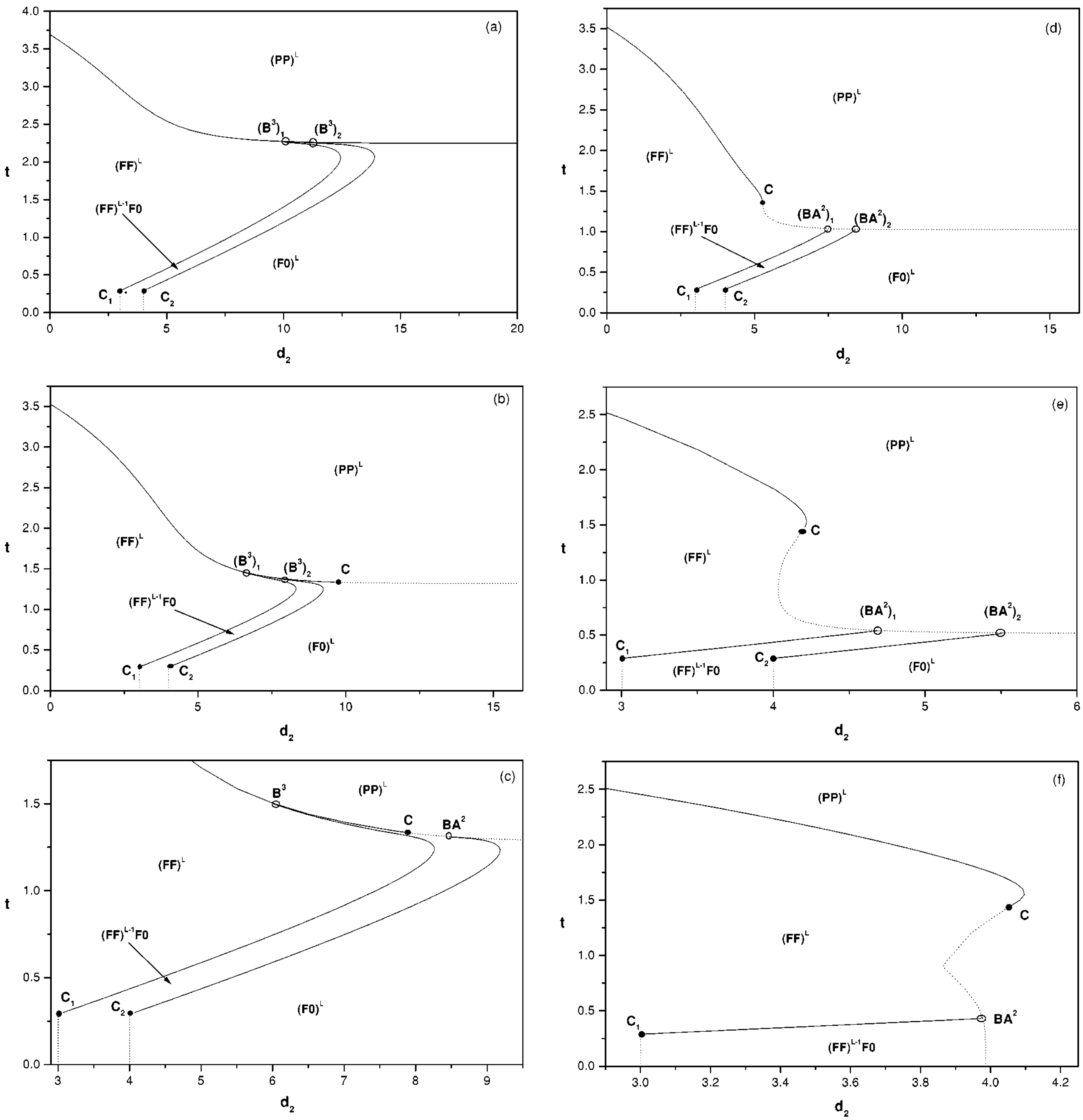

FIG. 2. The phase diagrams in the (t,d_2) plane for a generic even value of N $(N=6)$ and generic values of d_1. (a) $d_1=1$, (b)$d_1=1.85$, (c) $d_1=1.855$, (d) $d_1=1.9$, (e) $d_1=1.99$, (f) $d_1=2.01$, (g) $d_1=2.1$, (h) $d_1=2.25$, (i) $d_1=2.75$, (j) $d_1=3.5$, (k) $d_1=3.8$, (l) $d_1=3.9$, (m) $d_1=4.01$, (n) $d_1=4.1$, (o) $d_1=5$. The solid lines are of second order, the doted ones are of first order. Filled circles are tricritical points while empty circles are the other multicritical points and end points.

order and n of first order; the multicritical point C denotes the intersection of m lines of second order; the tricritical point, which is the intersection of a line of second order and a line of first order, is denoted in particular by C. The tricritical points will (as is common) be represented in the figures by filled circles while the end points and the multicritical points will be represented by empty ones. In addition, the following notations of the different phases will be adopted: $(FF)^L$ is, for example, a state where all the layers are in the ferromagnetic state, i.e., the magnetization and the quadrupolar moment of each layer are both different from zero. $(FF)^{L-1}F0$ is a phase where all the layers are in the ferromagnetic state except the last one which is in the nonmagnetic state (denoted by 0) and is characterized by vanishing magnetization and quadrupolar moment. $(PP)^L$ is a phase where all the layers are in the paramagnetic state, i.e., the magnetization of each layer is equal to zero but not the quadrupolar moment.

For an even number of layers $(N=2L)$, 15 types of topology of the phase diagram in the (t,d_2) plane are found.

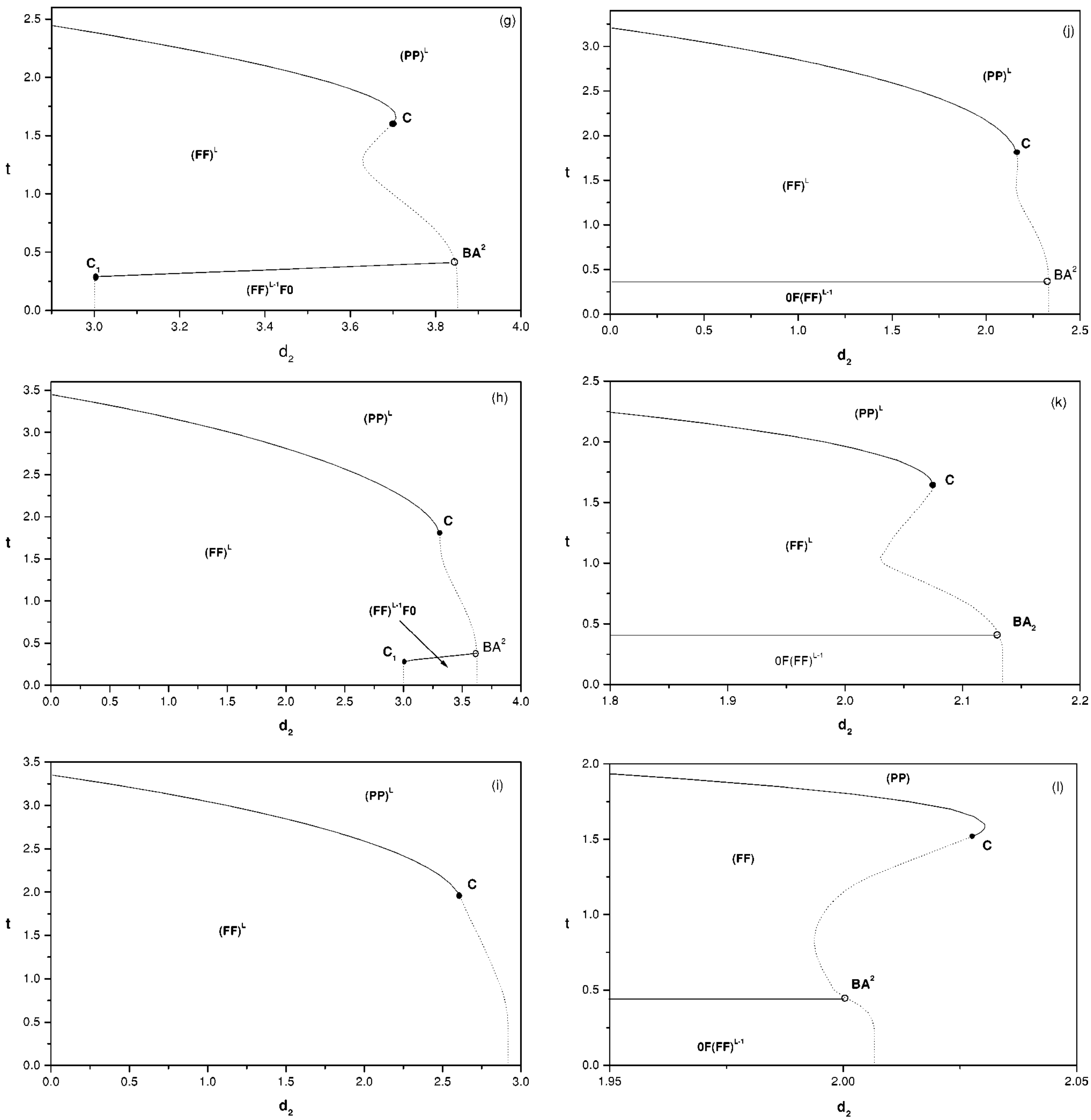

FIG. 2. (*Continued*).

They may be gathered into six groups, each one is characterized by a certain range of variation of d_1.

(1) For $0<d_1<d_{trc}^{(2)}$ [e.g., Fig. 2(a)], there is a critical line separating the paramagnetic phase $(PP)^L$ from the ferromagnetic ones $(FF)^L$, $(FF)^{L-1}F0$, and $(F0)^L$. These ferromagnetic phases are separated by two transition lines of first order at low temperatures which meet two critical lines at two tricritical points (totally inside the ordered phases) C_1 and C_2, respectively. The first-order lines reach the d_2 axis at the fixed values (independent of L) $d_2=3$ and $d_2=4$ respectively. The critical lines present both a reentrant behavior near the paramagnetic-ferromagnetic (P-F) transition line and meet this last at two multicritical points $(B^3)_1$ and $(B^3)_2$ respectively. The topology described here is characterized, contrary to the ordinary Blume-Capel model, by the absence of a tricritical point in the (P-F) transition line . The value of d_1 over which this point appears is found to be $d_{trc}^{(2)}=1.848$. This is equal to 8 ln 2/3 which is the analytic mean-field theory expression of the tri-critical crystal field of the spin-1 Blume-Capel square lattice.

(2) For $d_{trc}^{(2)}<d_1<2$, four types of topology are found with increasing d_1, all of them present a tricritical point in the P-F transition line and present the same features of the type-1 topology with some differences. For d_1 in the vicinity of $d_{trc}^{(2)}$ the lines of transition (F-F lines) separating the ferromagnetic phases $(FF)^L$, $(FF)^{L-1}F0$, and $(F0)^L$ still ex-

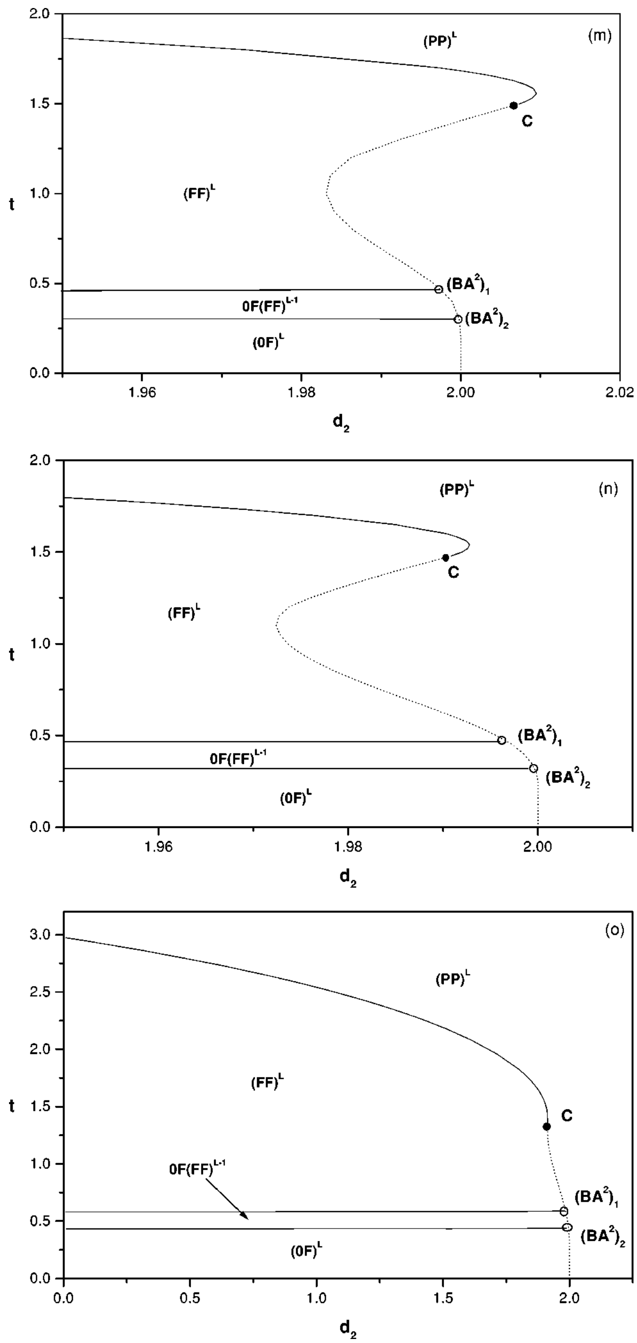

FIG. 2. (*Continued*).

hibit the reentrant phenomenon near the P-F transition line and meet this one at the multicritical points $(B^3)_1$ and $(B^3)_2$ [e.g., Fig. 2(b)]. With increasing d_1, the F-F lines meet the P-F line at the multicritical point B^3 and at the critical end-point BA^2 respectively, and still present the reentrant behavior [e.g., Fig. 2(c)]; for higher values of d_1, the former lines lose the reentrant behavior and meet the P-F line at two distinct critical end points $(BA^2)_1$ and $(BA^2)_2$ as is depicted in Fig. 2(d). Finally, for d_1 close to 2 the P-F first-order line develops a reentrant topology [e.g., Fig. 2(e)].

Note that for $d_1<2$ the ferromagnetic phase $(F0)^L$ is stable for an infinitely large value of d_2 at temperatures lower than a temperature $t_c^{(2)}(d_1)$ which is independent of the number of layers $2L$. $t_c^{(2)}(d_1)$ is but the critical temperature of the ordinary two-dimensional spin-1 Blume-Capel model corresponding to d_1. This may easily be understood even beyond the mean-field approximation. In fact at low temperatures and for large values of d_2, the odd layers are all nonmagnetic ($m_{2k+1}=0$) and the system of equations of the magnetizations m_{2k} of the even layers is decoupled to L equivalent two-dimensional equations with a crystal field d_1: the magnetizations m_{2k} (and then the total magnetization) vanish at the same temperature which is $t_c^{(2)}(d_1)$. For $d_1>2$ the ferromagnetic phase is unstable for large values of d_2, as will be seen, in accordance with the ground-state phase diagram.

(3) For $2<d_1<3-1/L$, three types of topology exist. For these topologies the ferromagnetic state $(F0)^L$ disappears from the ordered phases. The ferromagnetic phases $(FF)^L$ and $(FF)^{L-1}F0$ are, as above, separated by a transition line of first order, at low temperatures, which reaches the d_2 axis at $d_2=3$ and meets the second order line at a tricritical point C_1. This last line meets the P-F line at a critical end-point BA^2. For d_1 in the close vicinity of 2, the P-F line of transition exhibits a reentrant and double-reentrant behaviors [e.g., Fig. 2(f)]; with increasing d_1, only the double reentrant still exist [e.g., Fig. 2(g)] and then it disappears for higher values of d_1 [e.g., Fig. 2(h)]. Note that the P-F transition line reaches, for $2<d_1<3-1/L$, the d_2 axis at d_2 given by $(L-1)d_2=(6L-4)-Ld_1$: the surface of the $(FF)^{L-1}F0$ phase then decreases with increasing d_1 and it collapses at $d_1=3-1/L$.

(4) For $3-1/L<d_1<3$, the phase diagram is of the same type as that of the ordinary spin-1 Blume-Capel model [e.g., Fig. 2(i)]; the first-order line reaches the d_2 axis at d_2 given by $d_2=(6-1/L)-d_1$.

(5) For $3<d_1<4$, three types of topology are found. These are characterized by the appearance of the ferromagnetic phase $0F(FF)^{L-1}$ at low temperatures. The ferromagnetic phases $(FF)^L$ and $0F(FF)^{L-1}$ are separated by a critical line of approximately constant temperature which meets the P-F transition line at a critical end-point BA^2. The P-F line reaches the d_2 axis at d_2 given by $Ld_2=(6L-4)-(L-1)d_1$. For d_1 far from 4, a typical phase diagram is given in Fig. 2(j). With increasing d_1, the P-F transition line develops a double-reentrant behavior [e.g., Fig. 2(k)], and when d_1 approaches 4 this line presents a reentrant and double-reentrant behaviors [e.g., Fig. 2(l)].

(6) For $d_1>4$, three types of topology are fond; these are characterized by the appearance, in addition to the state $0F(FF)^{L-1}$, of the state $(0F)^L$ at low temperatures. The ferromagnetic phases $(FF)^L$, $0F(FF)^{L-1}$ and $(0F)^L$ are separated by two critical lines of approximately constant temperatures which meet the P-F transition line at two critical end points $(BA^2)_1$ and $(BA^2)_2$, respectively. The P-F line reaches the d_2 axis at $d_2=2$. For values of d_1 very close to 4 the P-F line presents a reentrance and a double reentrance [e.g., Fig. 2(m)]; the reentrance disappears with increasing d_1 [e.g., Fig. 2(n)] and then the double reentrance disappears for high values of d_1 [e.g., Fig. 2(o)].

For an odd number, $N=2L+1$, of layers, the ground-state [Fig. 1(b)] has only five different phases (instead of six for N even); in fact, for small values of d_1 ($d_1<2$) only two phases now exist: $(11)^L 1$ (for $d_2<4$) and $(10)^L 1$ (for $d_2>4$).

For finite temperatures, 14 types of topology exist in this case.

(i) For $0<d_1<d_{trc}^{(2)}$ the topology is like the type-1 above (in the case of an even number of layers) but with only two ferromagnetic phases $(FF)^L F$ and $(F0)^L F$ separated by a unique line having a tricritical point C_1 at low temperatures.

(ii) For $d_{trc}^{(2)}<d_1<2$ there are four types of topology which are like those of the group 2 above, but with the modification mentioned in i).

(iii) For $2<d_1<3$, there are no topologies like those of the group 3 above. The topologies, in the number of three, are all of the ordinary Blume-Capel type, but for the two first ones (d_1 close to 2) the P-F transition line develops a reentrance for d_1 very close to 2, and a reentrance and double-reentrance for higher values of d_1 (Fig. 3).

(iv) For $3<d_1<4$, there are three types of topology which are like those of the group 5 above, but with the ferromagnetic phase $0F(FF)^{L-1}0$ at low temperatures [instead of $0F(FF)^{L-1}$ for N even].

(v) For $d_1>4$, there are three topologies which are like those of the group 6 above, but with the ferromagnetic phases $(0F)^L 0$ and $0F(FF)^{L-1}0$ at low temperatures [instead of $(0F)^L$ and $0F(FF)^{L-1}$ for N even].

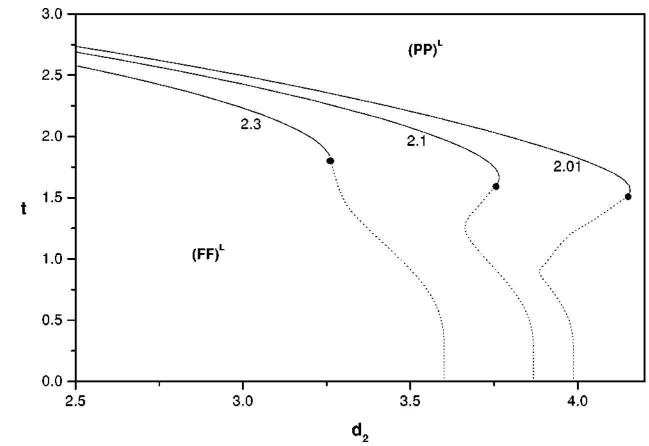

FIG. 3. The phase diagram in the (t,d_2) plane for a generic odd value of N ($N=7$) and generic values of d_1 in the range $2<d_1<3$. The number accompanying each curve is the value of d_1. The solid lines are of second order, the doted ones are of first order.

IV. CONCLUSION

We have studied, using mean-field theory, the phase diagrams of a ferromagnetic spin-1 Blume-Capel film with an alternating crystal field: $\Delta=\Delta_1$ on the odd layers and $\Delta=\Delta_2$ on the even ones. The ground-state phase diagrams in the (d_1,d_2) plane ($d_1=\Delta_1/J$ and $d_2=\Delta_2/J$) are determined analytically; the number of their phases depends on the parity of the number of layers of the film. At finite temperatures, fifteen types of topology, depending on the range of variation of d_1, are found in the (t,d_2) plane for an even number of layers, but only fourteen for an odd number of layers. The phase diagrams exhibit many multicritical points. In particular, a tricritical point C appears in the paramagnetic-ferromagnetic line of transition, but only for values of d_1 larger than a threshold value $d_{trc}^{(2)}$ which is but the mean-field tricritical crystal field of the spin-1 Blume-Capel model on a square lattice. Moreover, lines of transition presenting the reentrant and double-reentrant behaviors also appear in the phase diagrams.

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[1] M. Blume, Phys. Rev. **141**, 517 (1966).
[2] H.W. Capel, Physica (Amsterdam) **32**, 966 (1966).
[3] D. Mukamel and M. Blume, Phys. Rev. A **10**, 610 (1974).
[4] M. Blume, V.J. Emery, and R.B. Griffith's, Phys. Rev. A **4**, 1071 (1971).
[5] D.M. Saul and M. Wortis, in *Magnetism and Magnetic Materials—1971*, edited by C.D. Graham and J.J. Rhyne, AIP Conf. Proc. No. 5 (AIP, New York, 1972), p. 349; P.F. Fox and D.S. Gaunt, J. Phys. C **5**, 3085 (1972); D.M. Saul, M. Wortis, and D. Stauffer, Phys. Rev. B **9**, 4964 (1974).
[6] M. Tanaka and K. Takahashi, Phys. Status Solidi B **93**, K85 (1979).
[7] B.L. Arora and D.P. Landau, in *Magnetism and Magnetic Materials—1971*, edited by C.D. Graham and J.J. Rhyne, AIP Conf. Proc. No. 5 (AIP, New York, 1972), p. 352; A.K. Jain and D.P. Landau, Phys. Rev. B **22**, 445 (1980); W. Selk and J. Yeomans, J. Phys. A **16**, 2789 (1983); C.M. Care, *ibid.* **26**, 1481 (1993); M. Deserno, Phys. Rev. E **56**, 5204 (1997).
[8] A.N. Berker and M. Wortis, Phys. Rev. B **14**, 4946 (1976); T.W. Bukhard, *ibid.* **14**, 1196 (1976); H. Dickinson and J. Yeomas, J. Phys. C **16**, L345 (1983).
[9] C. Buzano and A. Pelizzola, Physica A **216,** 158 (1995).
[10] A. Benyoussef, N. Boccara, and M. Saber, J. Phys. C **19**, 1983 (1986).
[11] A. Benyoussef and H. Ez-Zahraouy, Phys. Scr. **57**, 603 (1998).
[12] L. Bahmad, A. Benyoussef, and H. Ez-Zahraouy, J. Magn. Magn. Mater. **251**, 115 (2002).
[13] A. Maritan, M. Cieplak, M.R. Swift, F. Toigo, and J.R. Banavar, Phys. Rev. Lett. **69**, 221 (1992); A. Benyoussef, T. Biaz, M. Saber, and M. Touzani, J. Phys. C **20**, 5349 (1987); T. Kaneyoshi and J. Mielnicki, J. Phys.: Condens. Matter **2**, 8773 (1990).
[14] T. Kaneyoshi, J. Magn. Magn. Mater. **92**, 59 (1990).
[15] R.B. Griffiths, Phys. Rev. B **12**, 345 (1975).
[16] We use natural notations for the model where the basic entity is a bilayer. A film of an even number of layers, $N=2L$, is viewed as built up L bilayers. The state $(10)^L$ denotes, for example, the state where the L bilayers of the film are all in the state (10) for which the first layer is in the state 1 (the spins of its sites are all equal to 1) and the second is in the state 0 (the spins of its sites are all equal to 0); $(10)^L=1010\ldots10$. In the same way, a film of an odd number of layers, $N=2L+1$, is viewed as built up L bilayers plus one single layer; $01(11)^{L-1}0$ denotes, for example, the state where the first bilayer is in the state (01), the $(L-1)$ following bilayers are all in the state (11) and the last single layer is in the state 0; $01(11)^{L-1}0=0111\ldots110$.