The Spin-S Blume–Capel RG Flow Diagram

S. Moss de Oliveira,[1] P. M. C. de Oliveira,[1] and F. C. de Sá Barreto[2]

Using the finite-size scaling renormalization group, we obtain the two-dimensional flow diagram of the Blume–Capel model for $S = 1$ and $S = 3/2$. In the first case our results are similar to those of mean-field theory, which predicts the existence of first- and second-order transitions with a tricritical point. In the second case, however, our results are different. While we obtain in the $S = 1$ case a phase diagram presenting a multicritical point, the mean-field approach predicts only a second-order transition and a critical endpoint.

KEY WORDS: Renormalization group; finite-size scaling; multicritical points.

1. INTRODUCTION

The finite-size scaling renormalization group (FSSRG) was introduced in ref. 1 and is based only on the finite-size scaling hypothesis,[2] with no further assumptions. Its main idea is to construct particular quantities scaling as L^0 in the thermodynamic limit $L \to \infty$, L being the linear size of the system. By preserving these quantities, independently of particular prescriptions relating states S of the largest lattice to S' of the smallest one, one obtains RG recursion relations without any conceptual problem. The construction of these quantities is based on the symmetries between the various ground states of the system. The FSSRG in its first version[1] was applied to study the Ising model in hypercubic lattices. More recently, using it to study the three-dimensional diluted Ising model, we were able to find a semiunstable fixed point in the critical frontier concentration p versus exchange coupling J,[3] characterizing a universality class crossover when one goes from pure to diluted Ising ferromagnets. Moreover, the

[1] Institute of Physics, Fluminense Federal University, Niterói, RJ, Brazil 24001-970. E-mail: GFIPMCO@BRUFF.bitnet or GFIPMCO@VMHPO.UFF.BR.
[2] Departamento de Física ICEX, Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brazil 30161-970. E-mail: SBARRETO@BRUFMG.bitnet or SBARRETO@FISICA.UFMG.BR.

specific heat exponents we obtained for the pure and diluted regimes are in agreement with the Harris criterion.[4] Based on such a success, we decided to use the FSSRG to study the two-dimensional spin-S Blume–Capel model.

The model is a simple generalization of the spin-1/2 Ising model, described by the Hamiltonian

$$\mathscr{H} = -J \sum_{\langle ij \rangle} S_i S_j + D \sum_i S_i^2 \tag{1}$$

where $J > 0$ and the spins S_i have values $-S$, $-S+1$,..., S, with $2S$ being an integer. The first sum is over all nearest-neighbor sites of the lattice and D is the parameter of anisotropy (single-ion anisotropy). For $S = 1$, $\mathscr{H}$ is a well-studied model introduced by Blume[5] and Capel[6] to describe critical–tricritical phenomena. On the temperature–anisotropy phase diagram the ordered ferromagnetic and the disordered paramagnetic regions are separated by a phase boundary which changes character at a tricritical point. According to mean-field calculations, the first-order transition line goes to zero at $D/zJ = 1/2$, where z is the coordination number. This result can also be exactly obtained by simple reasoning about the ground states (see Section 2). Several approximate schemes have been used to stablish the thermodynamic behavior of this model (see references in ref. 7). For arbitrary spin S, the model has been less studied. A recent mean-field solution[7] of the general spin-S Blume–Capel model shows that for integer spins there exist one tricritical point and a disordered phase at low temperature which are not present for semi-integer spins. There exists at $T = 0$ a multiphase point from which a number of first-order boundaries spread out. In particular, for the spin-3/2 model there is one first-order line ending at an isolated critical point, inside the ordered ferromagnetic region. In the following section we analyze the model for $S = 1$. The various phase regions are qualitatively determined. In Section 3 we introduce the method. A more detailed description can be found in ref. 3. In Section 4 we present the results for the flow diagram for the $S = 1$ and $S = 3/2$ models in the two-dimensional square lattice. Finally, in Section 5 we present some concluding remarks.

2. ANALYSIS FOR $S = 1$

Before explaining the FSSRG method, it is interesting to investigate what information can be extracted in advance from the Hamiltonian. We start rewriting Eq. (1) as

$$-\mathscr{H} = J \sum_{\langle ij \rangle} S_i S_j + \mathscr{D} \sum_i \sigma_i \tag{2}$$

where $S_i = +1$, 0, or -1, $\sigma_i = 2S_i^2 - 1 = +1$ or -1, and $\mathscr{D} = -D/2$. It is easy to verify that these two Hamiltonians are equivalent up to an additive constant. The following information can be obtained from Eq. (2):

(i) *The symmetry* $J \leftrightarrow -J$. Dividing the lattice into two sublattices (chessboard), inverting all the spins of one sublattice, and changing the sign of J, the system remains invariant. That is, the ferromagnetic order is symmetric to the antiferromagnetic one. Therefore, it is enough to study the $J \geqslant 0$ half of the phase diagram.

(ii) *The limit when the temperature* $T \to 0$ *with* $\mathscr{D} < 0$. In this limit the system is in one of its three possible ground states, one corresponding to all spins $S_i = 1$, the other to all $S_i = -1$, and the third one to all spins $S_i = 0$. For the first and second ground states the Hamiltonian per site can be written as

$$-\mathscr{H}_F/N = 2J + \mathscr{D} \tag{3}$$

where the factor 2 corresponds to the ratio (number of bonds)/(number of sites) for a square lattice. For the third ground state (all $S_i = 0$) the Hamiltonian per site is given by

$$-\mathscr{H}_Z/N = -\mathscr{D} \tag{4}$$

It is important to understand that the two former ground states correspond to a usual ordered ferromagnetic phase with a nonzero magnetization. The third ground state, however, corresponds to an ordered phase, but with zero magnetization, with the majority of the spins equal to zero. A first-order transition will occur for $\mathscr{H}_F = \mathscr{H}_Z$, that is,

$$2J + \mathscr{D} = -\mathscr{D} \Rightarrow J + \mathscr{D} = 0 \tag{5}$$

In this way the phase diagram J/T versus $\mathscr{D}/T$ in the limit J, $-\mathscr{D} \to \infty$ corresponds to a straight line given by $J/T + \mathscr{D}/T = 0$. For $(J/T + \mathscr{D}/T) > 0$ the system is in the usual ferromagnetic phase, and for $(J/T + \mathscr{D}/T) < 0$ it is in the "zero phase" mentioned above. This result is also reproduced within mean-field theory.[5-7]

(iii) *The limit* $\mathscr{D} \to \infty$. In this case $S_i = +1$ or -1, and on this Ising limit we find $J_c = (1/2)\ln(\sqrt{2} + 1) = 0.4407$ and $\nu = 1$ for the critical coupling and correlation length exponent, respectively. Hereafter, we take $T = 1$ for simplicity.

(iv) *The limit* $J \to 0$. In this limit the spins are independent and we can write

$$Z = Z_i^N = (2e^{\mathscr{D}} + e^{-\mathscr{D}})^N \propto (e^{\mathscr{D} + (1/2)\ln 2} + e^{-\mathscr{D} - (1/2)\ln 2})^N$$

Therefore there is a "transition" from the zero phase to a paramagnetic phase when $\mathscr{D} + 1/2 \ln 2 = -\mathscr{D} - 1/2 \ln 2$, that is, $\mathscr{D}_c = -1/2 \ln 2 = -0.3466$. This is a phase transition induced by an external field, and corresponds to no singularities in the thermodynamic quantities. Since both phases have zero magnetization, they cannot be distinguished through a mean-field approach, which usually measures the magnetization to identify the different phases of the system.

3. THE METHOD

One of the most important advantages of the FSSRG is that one does not need to adopt any particular recipe of the type

$$\exp[-\mathscr{H}'(S')/T] = \sum_{S} P(S, S') \exp[-\mathscr{H}(S)/T]$$

relating the spin states S of the original system to the spin states S' of a renormalized system. In traditional real-space renormalization group (RSRG) implementations, the choice of a particular weight function $P(S, S')$, e.g., the so-called majority rule, is generally based on plausibility arguments, and involves uncontrollable approximations. Based on this weakness, many criticisms have been made about RSRG since its introduction 20 years ago.[4] In spite of these criticisms, RSRG has been an important investigation tool since then. On the other hand, FSSRG is free from these criticisms and shares with RSRG some good features, such as the possibility of extracting *qualitative* information from *multiparameter RG flux diagrams*, including crossovers, universality classes, universality breakings, multicriticalities, orders of transitions, etc. Other unpleasant consequences of particular weight functions, such as the so-called proliferation of parameters, are absent from FSSRG.

In order to explain the method, we will consider a d-dimensional hypercubic lattice with its cover and bottom $(d-1)$-dimensional hypersurfaces. There are two quantities to be preserved in the renormalization process: the magnetic quantity $\mathscr{D}$ and the thermal quantity $\mathscr{T}$. The first one is defined by

$$\mathscr{D} = \left\langle \text{sign}\left(\sum_{i} \sigma_i\right) \right\rangle \tag{6}$$

where $\langle \cdots \rangle$ means the canonical thermodynamic average, and $\text{sign}(x) = -1, 0,$ or $+1$ for $x < 0, x = 0,$ and $x > 0$, respectively. This quantity is referred to as a magnetic quantity because it has a nonzero value only in the presence of a magnetic field (which in this model is the field $\mathscr{D}$). In

this way it is related to the symmetry breaking of the system. The other quantity is defined, through the surfaces of the lattice, as

$$\mathscr{T} = \langle \mu(\text{top}), \mu(\text{bottom}) \rangle \tag{7}$$

where $\mu = +1$ if the majority of the spins $S_i = +1$, $\mu = 0$ if the majority of the spins $S_i = 0$, and $\mu = -1$ if the majority of the spins $S_i = -1$. That is, the quantity $\mathscr{T}$ is related to the sign of the majority of the spins of the top and bottom hypersurfaces. There are three possible values of μ because there are also three different possible ground states. If we were studying the Ising model ($S_i = \pm 1/2$), for instance, we should admit only two possible values for μ. As extensively explained in ref. 3, the quantity $\mathscr{T}$ is related to ergodicity or long-range order breaking. It vanishes above T_c (paramagnetic phase) and equals 1 below T_c (ordered phase) independently of the existence of a magnetic field. Another point which is also carefully discussed in ref. 3 is the zero value of the anomalous dimension ϕ of both $\mathscr{Q}$ and $\mathscr{T}$, which is a consequence of their definition. Just because $\phi = 0$ we can guarantee that these quantities scale as L^0 and so are preserved during the renormalization process.

4. THE LATTICES AND RESULTS

4.1. Results for $S = 1$

In Fig. 1 we show the lattices we have used. In fact, these are the smallest ones that could be chosen for a renormalization process. Usually the best way to respect the ratio (number of bonds)/(number of sites) = 2 of the infinite square lattice when using finite lattice approximations is to adopt periodic boundary conditions. However, for such tiny lattices, it is
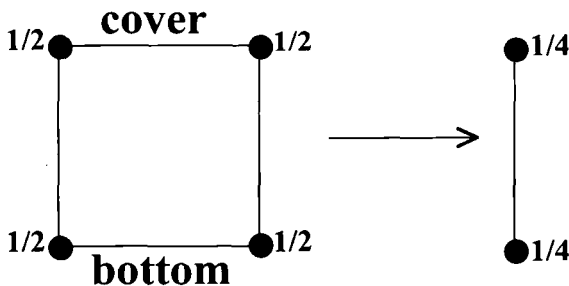

Fig. 1. The lattices used in the renormalization process and the weights attributed to the sites. Also the cover and bottom surfaces are indicated for this square lattice case.

more convenient to attribute weights to the sites according to their coordination number[9] as shown in Fig. 1. The corresponding renormalization group equations are of the form

$$\mathcal{Q}_{L'}(J', \mathcal{D}') = \mathcal{Q}_L(J, \mathcal{D}) \tag{8a}$$

and

$$\mathcal{T}_{L'}(J', \mathcal{D}') = \mathcal{T}_L(J, \mathcal{D}) \tag{8b}$$

where the primes are referred to the smallest lattice of size L'.

In Fig. 2 we show the resulting flow diagram. The attractors of the different phases are represented by squares, critical points by dots, and the tricritical point by a star. The full line is a second-order critical frontier, the dashed line is a first-order one, and the dotted line, as mentioned before, separates the usual paramagnetic phase from the "zero phase."

The critical point at the upper part of the diagram $(\mathcal{D} \to \infty)$ is related to the analysis made in Section 2(iii), and at this point we have found $J_c = 0.4730$. It is important to note that we are mainly interested in the qualitative features of the phase diagrams, and that with so tiny lattices it would not make sense to compare our numerical results to those obtained, for instance, through Monte Carlo calculations or conformal invariance arguments.[10] Nevertheless, any predefined numerical accuracy can be
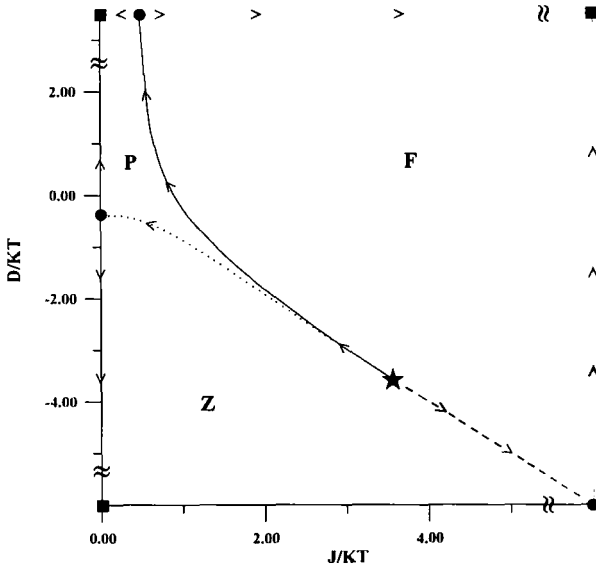

Fig. 2. The FSSRG flow diagram for $S = 1$.

obtained through the present method, simply by using large enough lattices. One can, for instance, calculate the quantities $\mathscr{D}$ and $\mathscr{T}$ through Monte Carlo sampling.[1]

The critical point at $J = 0$ is related to Section 2(iv), and we have found $\mathscr{D}_c = 0.3478$. At the tricritical point we have obtained $J_T = 3.5836$ and $\mathscr{D}_T = -3.5830$, in agreement with the analysis made in Section 2(ii).

Considering b the scaling factor and d the dimension of the system, we can characterize a first-order transition by the magnetic eigenvalue $\lambda = b^d$ calculated at the attractor of the critical line, that is, at the critical point that can be seen at the lower right corner of our phase diagram $(J, -\mathscr{D} \to \infty)$. Taking the limit $T \to 0$ $(\mathscr{D} < 0)$ in our RG equations, we have found $\lambda = 4 = b^d$, which ensures that the dashed line represents in fact a first-order transition.

4.2. Results for $S = 3/2$

In this case the Hamiltonian can also be represented by Eq. (2), but now with $\sigma_i = (S_i^2 - 5/4) = +1$ or -1 for $S_i = \pm 3/2$ and $S_i = \pm 1/2$, respectively. The same analysis made for the $S_i = 1$ case can be easily performed again, and also the same calculation method can be applied. The
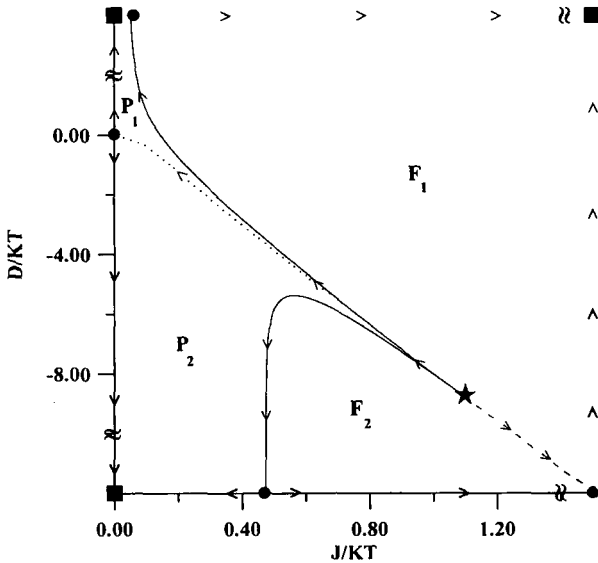

Fig. 3.   The FSSRG flow diagram for $S = 3/2$.

resulting RG flow diagram is shown in Fig. 3. The phases F_1 and P_1 are related to $S_i = \pm 3/2$, and F_2 and P_2 to $S_i = \pm 1/2$. Again for the magnetic eigenvalue calculated at the lower right critical point of the diagram we have $\lambda = 4 = b^d$, indicating the first-order character of the dashed critical line. At the upper left critical point $(\mathscr{D} \to \infty)$ we have found $J_c = 0.0525$, and at the $J = 0$ critical point, $\mathscr{D}_c = 0$. At the tetracritical point we have $J_T = 1.0967$ and $\mathscr{D}_T = -8.7831$. The lower critical point obtained for $\mathscr{D} \to -\infty$ is again the Ising spin-1/2 Onsager value, and we get $J_c = 0.4730$.

5. CONCLUDING REMARKS

In summary, we have calculated the flow diagram of the general spin-S Blume–Capel model for $S = 1$ and $S = 3/2$ by means of the FSSRG. For the $S = 1$ case the results reproduce previous calculations based on mean-field approximation as well as other approaches (see ref. 7 and references therein). For the spin-3/2 case new features are presented. The flow diagram for this case, as far as we know, has never been shown before. In addition, contrary to mean-field results,[7] we show the appearance of a tetracritical point in the phase diagram instead of an isolated critical endpoint. We remark that the numerical values obtained in these calculations are not accurate enough, due to the fact we have used small lattices to implement the renormalization process. However, the results are expected to be qualitatively correct and improved quantitative values can be obtained by the use of larger lattice cells. Finally, the same procedure can be applied for other values of spin S. We expect similar qualitative behavior as obtained here.

ACKNOWLEDGMENTS

REFERENCES

1. P. M. C. de Oliveira, *Europhys. Lett.* **20**:621 (1992).
2. M. E. Fisher, in *Proceedings of the International Summer School Enrico Fermi, Course LI, Critical Phenomena*, M. S. Green, ed. (Academic Press, 1971).
3. J. Monteiro de F. Neto, S. Moss de Oliveira, and P. M. C. de Oliveira, *Physica A* **206**:463 (1994).
4. A. B. Harris, *J. Phys. C* **7**:1671 (1974).
5. M. Blume, *Phys. Rev.* **141**:517 (1966).

6. H. W. Capel, *Physica* **32**:96 (1966); **33**:295 (1967); **37**:423 (1967).
7. J. A. Plascak, J. G. Moreira, and F. C. Sá Barreto, *Phys. Lett. A* **173**:360 (1993).
8. Th. Niemeijer and J. M. J. van Leeuwen, *Phys. Rev. Lett.* **31**:1411 (1973).
9. R. R. dos Santos, *J. Phys. C* **18**:L-1067 (1985).
10. D. Sen, *Phys. Rev. B* **44**:2645 (1991); A. L. Malvezzi, *Braz. J. Phys.* **24**:508 (1994).