The Spin-S Blume-Capel RG Flow Diagram

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Abstract

Using the Finite Size Scaling Renormalisation 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 end point.

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I - Introduction

The Finite Size Scaling Renormalisation Group (FSSRG) was introduced in [1], and it 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 semi-unstable 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 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

\[
\mathcal{H} = -J \sum_{<i,j>} S_i S_j + D \sum_i S_i^2 ,
\]

where \( J > 0 \) and the spins \( S_i \) have values \(-S, -S+1, \ldots, S\), 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 \( S = 1 \), \( \mathcal{H} \) 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 reasonings about the ground states (see section II). Several approximate schemes have been used to establish the thermodynamic behavior of this
model (see references in [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 analyse the model for $S = 1$. The various phase regions are qualitatively determined. In section III, we introduce the method. A more detailed description can be found in reference [3]. In section IV we present the results for the flow diagram for the $S = 1$ and $S = \frac{3}{2}$ models in the two dimensional square lattice. Finally, in section V, we present some concluding remarks.

II - Analysis for $S = 1$

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

$$-\mathcal{H} = J \sum_{\langle ij \rangle} S_i S_j + \mathcal{D} \sum_i \sigma_i,$$

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

i) The symmetry $J \leftrightarrow -J$

Dividing the lattice in 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 $J \geq 0$ half of the phase diagram.

ii) The limit when the temperature $T \to 0$ with $\mathcal{D} < 0$
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

$$-\mathcal{H}_F/N = 2J + D \quad ,$$

(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:

$$-\mathcal{H}_Z/N = -D \quad .$$

(4)

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

$$2J + D = -D \quad \Rightarrow \quad J + D = 0 \quad .$$

(5)

In this way the phase diagram $J/T$ versus $D/T$, in the limit $J, -D \to \infty$ corresponds to a straight line given by $J/T + D/T = 0$. For $(J/T + D/T) > 0$ the system is in the usual Ferromagnetic phase, and for $(J/T + D/T) < 0$ it is in the “Zero phase” mentioned above. This result is also reproduced within mean field theory [5,6,7].

**iii)** The limit $D \to \infty$

In this case $S_i = +1$ or $-1$, and on this Ising limit we shall 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

$$Z = Z_i^N = (2e^D + e^{-D})^N \propto (e^D + (1/2) \ln 2 + e^{-D} - (1/2) \ln 2)^N \quad .$$
Therefore there is a “transition” from the Zero phase to a Paramagnetic phase when $\mathcal{D} + 1/2 \ln 2 = -\mathcal{D} - 1/2 \ln 2$, that is $\mathcal{D}_c = -1/2 \ln 2 = -0.3466$. This is a phase transition induced by an external field, and corresponds to no singularities in the thermodynamic quantities. Since both phases have zero magnetisation, they cannot be distinguished through a mean field approach which usually measures the magnetisation to identify the different phases of the system.

III - 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

$$\exp(-\mathcal{H}'(S')/T) = \sum_S P(S, S') \exp(-\mathcal{H}(S)/T),$$

relating the spin states $S$ of the original system to the spin states $S'$ of a renormalised system. In traditional Real Space Renormalisation 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 twenty years ago [H]. 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 as, for instance, the possibility of extracting qualitative informations from multiparameter RG flux diagrams, including crossovers, universality classes, universality breakings, multicriticalities, orders of transitions, etc. Other unpleasant consequences of particular weight functions, 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 renormalisation process: the magnetic
quantity $Q$ and the thermal quantity $T$. The first one is defined by

$$Q = \left\langle \text{sign} \left( \sum_i \sigma_i \right) \right\rangle,$$

(6)

where $\langle ... \rangle$ 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 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 $D$). 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

$$T = \left\langle \mu(\text{top}) \mu(\text{bottom}) \right\rangle,$$

(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 $T$ is related to the sign of the majority of the spins of the top and bottom hypersurfaces. There are three possible values of $\mu$ 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 $\mu$. As extensively explained in ref. [3], the quantity $T$ 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 $\phi$ of both $Q$ and $T$, 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 renormalisation process.

IV - The Lattices and Results

Results for $S = 1$

In Fig.1 are shown the lattices we have used. In fact, these are the smallest ones that could be chosen for a renormalisation process. Usually the best way
to respect the ratio (number of bonds)/(number of sites) = 2 of the infinite square lattice, when using finite lattices approximations, is to adopt periodic boundary conditions. However, for such tiny lattices, it is more convenient to attribute weights to the sites according to their coordination number [9] as shown in Fig.1. The corresponding renormalisation group equations are of the form

\[ Q_{L'}(J', D') = Q_L(J, D) \]  \hspace{1cm} (8a)

and

\[ T_{L'}(J', D') = T_L(J, D) \]  \hspace{1cm} (8b)

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

In Fig.2 it is shown 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 (\( D \to \infty \)) is related to the analysis made in section II-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 obtained through the present method, simply by using large enough lattices. One can, for instance, calculate the quantities \( Q \) and \( T \) through Monte Carlo sampling [1].

The critical point at \( J = 0 \) is related to section II-iv), and we have found \( D_c = 0.3478 \). At the tricritical point we have obtained \( J_T = 3.5836 \) and \( D_T = -3.5830 \), in agreement with the analysis made in section II-ii).

Considering \( b \) the scaling factor and \( d \) the dimension of the system, a
first order transition can be characterized 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 ($J, -D \to \infty$). Taking the limit $T \to 0$ ($D < 0$) in our RG equations we have found $\lambda = 4 = b^d$, which ensures that the dashed line represents in fact a first order transition.

**Results for $S = 3/2$**

In this case the Hamiltonian can also be represented by eq.(2), but now with $\sigma \equiv (S^2 - 5/4) = +1$ or $-1$ for $S = \pm 3/2$ and $S = \pm 1/2$, respectively. The same analysis made for the $S = 1$ case can be easily performed again, and also the same calculation method can be applied. The resulting RG flow diagram is shown in Fig.3. The phases $F_1$ and $P_1$ are related to $S = \pm 3/2$, and $F_2$ and $P_2$ to $S = \pm 1/2$. 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 ($D \to \infty$) we have found $J_c = 0.0525$, and at the $J = 0$ critical point, $D_c = 0$. At the tetracritical point we have $J_T = 1.0967$ and $D_T = -8.7831$. The lower critical point obtained for $D \to -\infty$ is again the Ising spin-1/2 Onsager value, and we get $J_c = 0.4730$.

**V - 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 [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. Besides, contrary to mean field results [7], we show the appearance of a tetracritical point in the phase diagram, instead of an isolated critical end point. We remark that the
numerical values obtained in these calculations are not accurate enough, due to the fact we have used small size lattices to implement the renormalisation process. However, the results are expected to be qualitatively correct and improved quantitative values can be obtained by the use of larger lattices cells. Finally, the same procedure can be applied for other values of spin-$S$. We expect similar qualitative behavior as obtained here.
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**Figure Captions**

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

Figure 2– The FSSRG flow diagram for $S = 1$.

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