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On the criticality of frustrated spin systems with noncollinear order

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Abstract

We analyse the universal features of the critical behaviour of frustrated spin systems with noncollinear order. By means of the field theoretical renormalization group approach, we study the 3D model of a frustrated magnet and obtain pseudo- ε expansions for its universal order parameter marginal dimensions. These dimensions govern accessibility of the renormalization group transformation fixed points, and, hence, define the scenario of the phase transition.

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1. Introduction

Remarkable progress achieved in the description of phase transitions and critical phenomena due to application of the renormalization group (RG) [1] ideas leads sometimes to the conclusion that all principal work in the field has been done, especially if universal features of criticality are addressed. This is certainly not true, if one goes beyond a description of the para-to-ferromagnetic phase transition in a standard N -vector model [2], which belongs to the universality class of the $O(N)$ -symmetric ϕ^4 theory. To give an example, a study of realistic systems often calls for account of a single-ion anisotropy [3], structural disorder [3] or frustrations [4] that might essentially change the critical behaviour. An account of this new physics still remains a challenging problem.

The theoretical RG description of the above-mentioned systems requires field theories of complicated symmetry with several couplings. In theory, the critical point corresponds to the fixed point of the RG transformations. Accessibility of the fixed point, along with the

Table 1. Marginal dimension N_{c_3} obtained within different RG methods. See the text for details of the methods.

Fixed 3D, resummed										
3 loops	6 loops		$\sim\varepsilon^2$		$\sim 1/N$		NPRG			
	[13]	[5] [6]	[14]	[15]	[15]	[16]	[17]	[18]	[19]	[7]
3.91(1)	6	6.4(4)	3.39	5.3(2)	5	3.24	4.8	4	5	5.1

(non-universal) initial conditions of the RG flow is governed by the so-called marginal field dimensions. These are universal and together with the critical exponents and amplitude ratios constitute intrinsic features of criticality. It is well established by now that the universal features of a second-order phase transition in the 3D N -vector model are not sensitive to the single-ion cubic anisotropy if $N < N_c^{\text{cub}}$ [3]. Neither are they changed upon a weak quenched dilution by a non-magnetic component if only [3] $N > N_c^{\text{dil}}$. Currently, there exists a good agreement between the numerical values of the marginal dimensions N_c^{cub} , N_c^{dil} calculated in numerous RG and MC studies [3, 9, 10]. However, this is not the case for the frustrated systems, where even more marginal dimensions have been found and their numerical values are still under discussion [4, 11].

The problem we want to raise in this report concerns the critical behaviour of the 3D frustrated spin systems with noncollinear order. The most common physical realizations of such systems are stacked triangular antiferromagnets (examples are given by CsMnBr₃, CsNiCl₃, CsMnI₃, CsCuCl₃, VCl₂, VBr₂) and helimagnets (Ho, Dy, Tb, β -MnO₂). In the former case, the noncollinear order is caused by frustration due to the triangular geometry of the underlying lattice, whereas in the latter one it is due to the competition of ferro- and antiferromagnetic interactions. Currently, there exists a large literature devoted to the subject, which results from more than 20 year long studies [4]. However, neither experimentally nor theoretically has an unanimous conclusion been drawn so far about the nature of the phase transition into the ordered state in these systems. Important physical quantities which are under discussion are the marginal dimensions of the models. In particular, when the model is generalized to describe N -component vectors [12] (physical systems mentioned above correspond to $N = 2, 3$), one finds a marginal dimension N_{c_3} below which the phase transition is of first-order, whereas for $N > N_{c_3}$ it is of second-order. Several variants of the perturbative RG expansions [5, 6, 13–16] and various truncations for the Wilson-like non-perturbative RG (NPRG) equations [7, 17–19] give different numerical estimates for N_{c_3} (see table 1). However, they all agree that such a dimension (along with two further marginal dimensions, N_{c_2} and N_{c_1} , see below) exists. In our study, we aim at performing a thorough analysis of these marginal dimensions by means of the pseudo- ε expansion⁵ [20]: the technique which is known to provide the most accurate results in the 3D perturbative RG approach.

The rest of the paper is organized as follows: in the next section, we formulate the model we are interested in and obtain the expansions for its marginal dimensions, section 3 is devoted to the numerical estimates on their basis, section 4 gives conclusions and outlook.

2. The model and the pseudo- ε expansion

An effective Hamiltonian of the model of frustrated magnets with an N -component order parameter reads [12]

⁵ For an application of the pseudo- ε expansion in determination of marginal dimensions see [9, 10].

$$\mathcal{H} = \int d^d x \left\{ \frac{1}{2} [(\nabla\phi_1)^2 + (\nabla\phi_2)^2 + m_0^2(\phi_1^2 + \phi_2^2)] + \frac{u_0}{4!} [\phi_1^2 + \phi_2^2]^2 + \frac{v_0}{4!} [(\phi_1 \cdot \phi_2)^2 - \phi_1^2 \phi_2^2] \right\}. \quad (1)$$

In (1), m_0, u_0, v_0 are bare mass and couplings and $\phi_i \equiv \phi_i(x)$ are N -component vector fields, representing the cosine and sine modes associated with the spin ordering. The noncollinear (chiral) ordering occurs for $u, v \geq 0$.

We sketch the fixed points (FPs) picture retrieved in the previous RG studies [12]. For the high field dimensions $N > N_{c_3}$ four FPs exist: the Gaussian, $u = v = 0$, G , the Heisenberg $u \neq 0, v = 0$, $O(2N)$ symmetric, H (both unstable for the space dimension $d = 3$), and two nontrivial FPs $u \neq 0, v \neq 0$ (with $u, v > 0$), chiral and antichiral C_+ and C_- . The FP C_+ is stable and governs the chiral second-order phase transition. With a decrease of N , the FPs C_+ and C_- merge at $N = N_{c_3}$ and disappear: only unstable FPs G and H are present for N just below N_{c_3} . Note that Pelissetto *et al* and Calabrese *et al* [5, 6] have claimed that, once resummed, the six loop β -functions obtained directly in $d = 3$ exhibit a new root—a new fixed point—below an extra marginal dimension of the field estimated at $N \sim 5.7$. According to these authors, this fixed point is neither analytically related to the Gaussian fixed point in $d = 4$ nor to the fixed point found at large N in $d = 3$. It should therefore be non-perturbative, although it is found within the perturbative framework. Thus, they claim that below this new marginal dimension, and in particular for $N = 2, 3$, the transition is again of second order. Note also that this scenario disagrees with the results obtained within the NPRG approach for which the transition is (very weakly) of first order for $N < N_{c_3}$. We will return to this point at the end of our report. As N is further decreased, the nontrivial FPs C_+ and C_- , existing above N_{c_3} reappear at $N \leq N_{c_2}$, but now in the $u > 0, v < 0$ quadrant and thus do not describe the chiral phase (they both have complex coordinates for N between N_{c_3} and N_{c_2}). Finally at $N = N_{c_1}$ one of the nontrivial FPs merges with the FP H and, with further decrease of N , passes to the quadrant $u > 0, v > 0$, still remaining unstable. The above picture is supported both by the perturbative RG approach (ϵ -expansion accompanied by subsequent resummation [14] or by a conjecture about the series behaviour [15], resummed expansion in terms of renormalized couplings in a 3D RG scheme [5, 6, 13], $1/N$ expansion [15, 16]) and the non-perturbative RG [7, 17–19].

Discrepancies between the values of the marginal dimensions N_{c_i} obtained so far within the perturbative RG (see table 1 for N_{c_3}) to a great extent are because the series used for their analysis were rather short [13–16] and in general are known to be asymptotic at best [1]. So it is very desirable to perform an estimate of the marginal dimensions on the basis of the expansions which, on the one hand would be of the highest order and, on the other hand, would possess better convergence properties. As we show below, these two goals are reached by applying the pseudo- ϵ expansion to the six-loop $d = 3$ RG β -functions obtained for the effective Hamiltonian (1) in [5].

The method consists in introducing an auxiliary parameter (τ) into the β -functions which allows us to separate contributions to the FPs from the loop integrals of different order [20]. This is achieved by multiplying a zero-loop term by τ and obtaining FP coordinates and, subsequently, all FP quantities of the theory as series in τ with final substitution $\tau = 1$. Starting from the six-loop $d = 3$ RG β -functions of [5] we get the expansions for the fixed point coordinates and derive for the marginal dimensions

$$N_{c_3} = 21.797\,959 - 15.620\,635\tau + 0.262\,060\tau^2 - 0.150\,930\tau^3 - 0.039\,165\tau^4 - 0.029\,721\tau^5 \quad (2)$$

$$N_{c_2} = 2.202\,041 - 0.379\,365\tau + 0.202\,166\tau^2 - 0.084\,951\tau^3 + 0.092\,744\tau^4 - 0.097\,961\tau^5 \quad (3)$$

$$N_{c_1} = 2.0 - 0.666\,667\tau + 0.145\,212\tau^2 - 0.094\,836\tau^3 + 0.099\,757\tau^4 - 0.112\,325\tau^5. \quad (4)$$

Expansions (2)–(4), derived directly at $d = 3$, can be compared with the corresponding $\varepsilon = 4 - d$ -expansions [14]

$$N_{c_3} = 21.80 - 23.43\varepsilon + 7.088\varepsilon^2 \quad (5)$$

$$N_{c_2} = 2.202 - 0.569\varepsilon + 0.989\varepsilon^2 \quad (6)$$

$$N_{c_1} = 2 - \varepsilon + 1.294\varepsilon^2. \quad (7)$$

Formulae (2)–(4) take into account three orders of perturbation theory more than the highest available $\varepsilon = 4 - d$ -expansions (5)–(7). Moreover, comparing (2)–(4) and (5)–(7) one sees that the expansion coefficients in the pseudo- ε series decay much faster and one may expect to get more convergent results on their basis. And indeed this is the case as we will see in the next section.

3. Numerical estimates of the marginal dimensions

The field theoretic RG expansions are known to have zero radius of convergence and different resummation techniques are used to make numerical estimates on their basis [1]. Here, we make use of the Padé analysis [21] to make an analytic continuation of the expansions for $\tau = 1$. On one hand, already this simple technique allows us to show essential features of the pseudo- ε expansion behaviour; on the other hand, it allows us to determine numerical values of the marginal dimensions with a sufficient accuracy. The results for the pseudo- ε expansion series (2)–(4) are given below in the form of Padé tables. There, a result of an $[M/N]$ Padé approximant is represented as an element of a matrix with the usual notation, e.g. the first row gives results of the mere summation of the series:

$$N_{c_3} = \begin{bmatrix} 21.798 & 6.177 & 6.439 & 6.288 & 6.249 & 6.220 \\ 12.698 & 6.435 & 6.344 & 6.236 & \frac{6.126}{1.318} & \\ 9.827 & 6.290 & 6.230 & \frac{6.182}{1.751} & & \\ 8.463 & 6.247 & \frac{6.155}{1.453} & & & \\ 7.695 & 6.217 & & & & \\ 7.220 & & & & & \end{bmatrix} \quad (8)$$

$$N_{c_2} = \begin{bmatrix} 2.202 & 1.823 & 2.025 & 1.940 & 2.033 & 1.935 \\ 1.878 & 1.955 & 1.965 & 1.984 & 1.985 & \\ 1.984 & 1.966 & \frac{1.948}{0.385} & 1.985 & & \\ 1.962 & 1.977 & 1.988 & & & \\ \frac{2.012}{2.586} & 1.986 & & & & \\ 1.960 & & & & & \end{bmatrix} \quad (9)$$

$$N_{c_1} = \begin{bmatrix} 2.0 & 1.333 & 1.479 & 1.384 & 1.483 & 1.371 \\ 1.500 & 1.453 & 1.421 & 1.432 & 1.431 & \\ 1.458 & \frac{1.032}{1.105} & 1.431 & 1.431 & & \\ 1.421 & 1.436 & 1.431 & & & \\ 1.446 & 1.432 & & & & \\ 1.415 & & & & & \end{bmatrix}. \quad (10)$$

Results shown by fractions indicate that the Padé approximant contained a pole for τ close to 1 (the denominator shows the value of τ for which the pole is obtained). These tables can be compared with the analogous tables for the ε -expansions (5)–(7):

$$N_{c_3} = \begin{bmatrix} 21.80 & -1.630 & 5.458 \\ 10.507 & 3.812 & \\ 7.505 & & \end{bmatrix} \quad (11)$$

$$N_{c_2} = \begin{bmatrix} 2.202 & 1.633 & 2.622 \\ 1.750 & 1.994 & \\ 2.514 & & \end{bmatrix} \quad (12)$$

$$N_{c_1} = \begin{bmatrix} 2 & 1 & 2.294 \\ 1.333 & 1.564 & \\ 1.813 & & \end{bmatrix}. \quad (13)$$

One certainly sees that the convergence properties of the pseudo- ε expansion are better in comparison with the ε -expansion (cf the convergence of the results along the main diagonal and those parallel to it: there the Padé analysis is known to provide the most reliable data [21]). One more feature of the expansions for N_{c_i} is evident when one compares tables (8)–(10): whereas the central elements of table (10) give a firm estimate for N_{c_1} : $[2/2] = [3/2] = [2/3] = 1.431$, such stable behaviour is not found in the corresponding Padé tables (8), (9) for N_{c_3} , N_{c_2} . Obviously, this different behaviour is connected with the different origin of the marginal dimensions N_{c_1} from one side, and N_{c_3} , N_{c_2} from the other side. Indeed, the dimension N_{c_1} corresponds to merging of the non-trivial and Heisenberg FPs after which the non-trivial FP continuously passes to the other quadrant of the u - v plane whereas dimensions N_{c_3} , N_{c_2} correspond to the coalescence and *disappearance* of two non-trivial FPs (see discussion at the beginning of section 2).

To make the numerical estimates on the base of Padé tables (8)–(10) we proceed as follows. For N_{c_3} we take on the main diagonal the highest Padé approximant with an estimate $[2/2] = 6.23$ and suppose that the deviations from an account of higher-order terms will not exceed the difference $[2/2] - [1/1] = 0.21$. For N_{c_2} we take the highest obtained estimates $[3/2] = [2/3] = 1.99$ considering a confidence interval as $[3/2] - [2/2] = 0.04$. Subsequently, for N_{c_1} the central value is given by $[3/2] = [2/3] = [2/2] = 1.43$ with a confidence interval $[2/2] - [1/1] = 0.02$. Finally, we get for the marginal dimensions

$$N_{c_3} = 6.23(21) \quad N_{c_2} = 1.99(4) \quad N_{c_1} = 1.43(2). \quad (14)$$

The above estimates include within the error bars *all* elements of corresponding Padé tables except of the inverse approximants $[0/N]$ (and the approximant $[5/0]$ of (9)) and therefore, the confidence intervals in (14) are rather overestimated.

Comparison of our estimate for N_{c_3} with the perturbative RG data of table 1 supports recent estimates [5, 6] $N_{c_3} \sim 6$. We also suggest that the essential difference between this estimate and the numbers obtained within ε - and $1/N$ -expansions [14–16] is because the last have not been estimated with comparative accuracy which was caused in particular by the shortness of the corresponding series⁶. Estimates of N_{c_2} available so far are due to the resummation of three-loop massive RG expansions [13] and of the ε^2 expansion [14] (6): $N_{c_2} = 1.96$ and $N_{c_2} = 2.03(1)$, correspondingly (see footnote 6). Together with the symmetry arguments

⁶ The confidence interval ± 0.01 found in the three-loop studies of [13] should be considered rather as an accuracy estimate of the calculation scheme, since the six-loop studies within the same perturbation technique [6] shift, e.g., the central value for N_{c_3} from 3.91 to 6.

[13] providing $N_{c_2} > 2$ our estimate suggests that the value of N_{c_2} should be located very close to 2. In particular, this means that corresponding scenario of appearance of the pair of non-trivial FPs which is governed by this marginal dimension might not be found in numerical calculations for $N = 2$. Dimension N_{c_1} has its counterpart [13] as the marginal dimension of the N -vector model with a single-ion cubic anisotropy: $N_{c_1} = N_c^{\text{cub}}/2$, see section 1. The last has been estimated by different methods. In particular, the Padé–Borel resummation of the series (4) gives [9] a number coherent with the other data [3] $N_{c_1} = N_c^{\text{cub}}/2 = 1.431(3)$. Comparison of this number with our estimate (14) based on a much less elaborate technique supports the reliability of the scheme chosen here.

4. Conclusions

The numerical values of the marginal dimensions that we obtain represent clearly an improvement of the preceding determinations performed by both the perturbative methods and the NPRG one. Once again the pseudo- ε expansion turns out to be very accurate and constitutes probably a new way to analyse the critical behaviour of 3D frustrated magnets. However, the principal question about the order of the phase transition in these systems for $N = 2, 3$ still remains open. Obviously, our studies are in coherence with the FP picture of the NPRG and perturbative RG approaches, where no stable FP are found in the region $N_{c_3} > N > N_{c_2}$ (however the difference between numerical value of N_{c_3} and typical numerical values found in the NPRG studies [7, 17–19] calls for a more detailed analysis). Nevertheless, the existence of the FP found recently in [5, 6] and claimed to describe criticality of these systems can neither be supported nor rejected by our perturbative approach. We think that one possible way to shed light on this problem is to try to follow an evolution of this FP with change of d in order to understand its origin at the upper critical dimension $d = 4$.

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Note added. After the completion of this work [22], we learned about ε^4 -results for N_{c_3} , N_{c_2} and a six-loop pseudo- ε result for N_{c_3} [23]. The five-loop ε -expansion improves the ε^2 data for $N_{c_3} = 6.1(6)$ but leads to the unphysical conclusion $N_{c_2} = 1.968(1) < 2$. The pseudo- ε expansion of [23] for N_{c_3} coincides with our formula (2), but we report higher numerical accuracy.

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