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Critical behavior of frustrated spin models with noncollinear order

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We study the critical behavior of frustrated spin models with noncollinear order, including stacked triangular antiferromagnets and helimagnets. For this purpose we compute the field-theoretic expansions at a fixed dimension to six loops and determine their large-order behavior. For the physically relevant cases of two and three components, we show the existence of a stable fixed point that corresponds to the conjectured chiral universality class. This contradicts previous three-loop field-theoretical results but is in agreement with experiments.

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The critical behavior of frustrated spin systems with noncollinear or canted order has been the object of intensive theoretical and experimental studies (see, e.g., Refs. 1 and 2). In spite of these efforts, the critical behavior of these systems is still unclear, with field-theoretic (FT) renormalization-group (RG) methods, Monte Carlo simulations, and experiments obtaining different results.

In physical magnets noncollinear order is due to frustration that may arise either because of the special geometry of the lattice, or from the competition of different kinds of interactions. Typical examples of systems of the first type are three-dimensional stacked triangular antiferromagnets (STA), where magnetic ions are located at each site of a three-dimensional stacked triangular lattice. Examples are ABX_3-type compounds, where A denotes elements such as Cs and Rb, B stands for magnetic ions such as Mn, Cu, Ni, and Co, and X for halogens as Cl, Br, and I. At the chiral transition, they may be modeled by using short-ranged Hamiltonians for N-component spin variables defined on a stacked triangular lattice as

$$\mathcal{H}_{\rm STA} = -J \sum_{\langle ij \rangle_{xy}} \vec{s}_i \cdot \vec{s}_j - J' \sum_{\langle ij \rangle_z} \vec{s}_i \cdot \vec{s}_j , \qquad (1)$$

where $J<0$, the first sum is over nearest-neighbor pairs within triangular layers (xy planes), and the second one is over orthogonal interlayer nearest neighbors. The condition $N \geqslant 2$ is essential to have noncollinear ordering. In these spin systems the Hamiltonian is minimized by noncollinear configurations, showing a 120° spin structure. Frustration is partially released by mutual spin canting, and the degeneracy of the ground-state is limited to global O(N) spin rotations and reflections. As a consequence, at criticality there is a breakdown of the symmetry from O(N) in the high-temperature phase to O($N-2$) in the low-temperature phase, implying a matrixlike order parameter. Frustration due to the competition of interactions may be realized in helimagnets where a magnetic spiral is formed along a certain direction of the lattice (see, e.g., Ref. 1). The rare-earth metals Ho, Dy, and Tb provide examples of such systems.

The critical behavior of two- and three-component frustrated spin models with noncollinear order is controversial. Many experiments (see, e.g., Refs. 1 and 2) are consistent with a second-order phase transition which should belong to a new (chiral) universality class. As shown experimentally in Ref. 3 for an XY STA, chiral and spin order occurs simultaneously. On the other hand, the most recent FT calculations suggest that these systems undergo (weak) first-order transitions that effectively appear as second-order ones in experimental work. Three-loop perturbative calculations at fixed dimension $d=3$ (Ref. 4) and within the framework of the ϵ expansion[5] indicate a first-order transition, since no stable chiral fixed points are found for $N=2$ and $N=3$. These three-loop analyses show the presence of a stable chiral fixed point only for $N>N_c$ with $N_c>3$: $N_c=3.91$ (Ref. 4) and $N_c=3.39$ (Ref. 5). However, one may think that the observed disagreement is due to the shortness of the available series.

Similar conclusions are reached in studies based on the continuous RG approach.[6] Note, however, that the practical implementation of this method requires an approximation and/or truncations of the effective action, such as the local potential approximation or the first few terms of the derivative expansion, which are expected to be effective when the critical exponent $\eta \ll 1$.

Monte Carlo simulations apparently give contradicting results.[1,7,8] Simulations of $\mathcal{H}_{\rm STA}$ (see, e.g., Ref. 1, and references therein) support a second-order phase transition with different critical exponents, although the numerical results are not in quantitative agreement among the different authors. Simulations of modified lattice spin systems[7] which, according to general universality ideas, should belong to the same universality class of the Hamiltonian (1), show instead a first-order transition.

For sufficiently large values of N, all theoretical approaches predict a second-order phase transition, but there are still substantial discrepancies between Monte Carlo and three-loop FT calculations (see the discussion of Ref. 9 for $N=6$).

All these considerations show that a satisfactory theoretical understanding has not yet been reached. It is not clear whether experiments are observing first-order transitions in disguise or field theory is unable to describe these rather complex systems.

FT studies of systems with noncollinear order are based on the O(N)×O(M) symmetric Hamiltonian[10,1]

$$\mathcal{H}=\int d^d x \left\{ \frac{1}{2}\sum_a \left[(\partial_\mu \phi_a)^2 + r\phi_a^2 \right] + \frac{1}{4!} u_0 \left(\sum_a \phi_a^2 \right)^2 + \frac{1}{4!} v_0 \sum_{a,b} \left[(\phi_a \cdot \phi_b)^2 - \phi_a^2 \phi_b^2 \right] \right\}, \tag{2}$$

where ϕ_a $(1 \leqslant a \leqslant M)$ are M sets of N-component vectors. We will consider the case $M=2$, that, for $v_0>0$, describes frustrated systems with noncollinear ordering such as STA's. Negative values of v_0 correspond to simple ferromagnetic or antiferromagnetic ordering, and to magnets with sinusoidal spin structures.[10]

For $N=2$, which is the case relevant for frustrated two-component spin models, an ϵ-expansion analysis indicates the presence of four fixed points: the Gaussian one, an XY fixed point, an O(4)-symmetric, and a mixed fixed point. Using nonperturbative arguments,[11] one can show that the XY fixed point is the only stable one[12] among them. However, the region relevant for frustrated models, $v_0>0$, is outside the domain of attraction of the XY fixed point, which would imply a first-order transition. Nevertheless, it is still possible that other fixed points are present in the region $v_0>0$, although they are not predicted by the ϵ expansion. For $N=3$, one may easily show the existence of an O(6) fixed point for $v_0=0$, which is expected to be unstable.[1] According to the three-loop analyses of Refs. 4 and 5 no other fixed points are found for $N=3$, which would imply that the transition is of first order as well.

In order to investigate the existence of new fixed points, we have considered the fixed-dimension perturbative approach, extending the three-loop series of Ref. 4 to six loops. As we shall see, the results of our six-loop analysis are somehow surprising, contradicting most of the earlier FT works. Indeed, the analysis of the longer series provides a rather robust evidence for the existence of a different stable fixed point in the XY and Heisenberg cases, with critical exponents that are in agreement with the experimental results.

In the fixed-dimension FT approach one expands in powers of the quartic couplings and renormalizes the theory by introducing a set of zero-momentum conditions for the two-point and four-point correlation functions. All perturbative series are finally expressed in terms of the zero-momentum four-point renormalized couplings u and v normalized so that, at tree level, $u \approx u_0$ and $v \approx v_0$. The fixed points of the theory are given by the common zeros of the β functions $\beta_u(u,v)$ and $\beta_v(u,v)$. In the case of a continuous transition, when $\xi \to \infty$, the couplings u,v are driven toward an infrared-stable zero u^*,v^* of the β functions. On the other hand, the absence of stable fixed points is usually considered as an indication of a (weak) first-order transition.

Since FT perturbative expansions are asymptotic, the resummation of the series is essential to obtain accurate estimates of the physical quantities. For this purpose we studied the large-order behavior of the expansion in $\overline{u}=3u/(16\pi R_{2N})$, where $R_K \equiv 9/(8+K)$, and $\overline{v}=3v/(16\pi)$ at fixed $z \equiv \overline{v}/\overline{u}$. For $z \equiv \overline{v}/\overline{u}$ fixed and $M=2$, the singularity of the Borel transform closest to the origin, $\overline{u}_b$, is given by

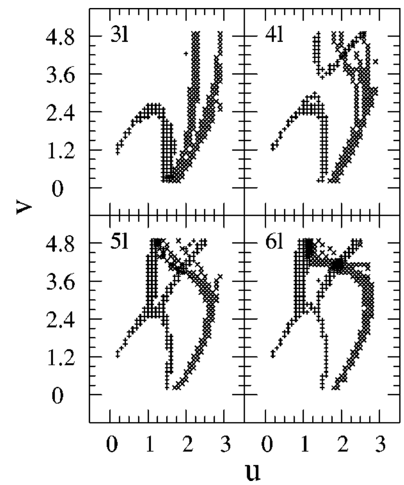

FIG. 1. Zeroes of the β functions for $N=2$ in the $(\overline{u},\overline{v})$ plane. Pluses (+) and crosses (×) correspond to zeros of $\beta_{\overline{u}}(\overline{u},\overline{v})$ and $\beta_{\overline{v}}(\overline{u},\overline{v})$, respectively.

$$\frac{1}{\overline{u}_b}=-aR_{2N} \qquad \text{for} \quad 4R_{2N}>z>0, \tag{3}$$

$$\frac{1}{\overline{u}_b}=-a\left(R_{2N}-\frac{1}{2}z\right) \qquad \text{for} \quad z<0, \qquad z>4R_{2N},$$

where $a=0.14777422\ldots$ and $R_K=9/(8+K)$. Moreover, we find that for $z>2R_{2N}$ the Borel transform has a singularity on the positive real axis, which, however, is not the closest one for $z<4R_{2N}$. Thus, for $z>2R_{2N}$ the series is not Borel summable.

In order to determine the fixed points we use the same method applied in Ref. 13 to the analysis of the RG functions of the cubic model. We resume the perturbative series by means of an appropriate conformal mapping[14] that takes into account the large-order behavior of the perturbative series at fixed z and turns the original series into a convergent sequence of approximations. To understand the systematic errors we vary two different parameters, b and α, in the analysis. We apply this method also for those values of z for which the series is not Borel summable. Although in this case the sequence of approximations is only asymptotic, it should provide reasonable estimates as long as $z<4R_{2N}$, since we are taking into account the leading large-order behavior.

In Figs. 1 and 2 we report our results for the zeros of the β functions, obtained from the analysis of the l-loop series, $l=3,4,5,6$. For each β function we consider 18 different approximants with $b=3,6,\ldots,18$ and $\alpha=0,2,4$ and we determine the lines in the $(\overline{u},\overline{v})$ plane on which they vanish. Then, we divide the domain $0 \leqslant \overline{u} \leqslant 4$ and $0 \leqslant \overline{v} \leqslant 5$ into 40×40 rectangles, marking those in which at least *two* approximants of each β function vanish. No fixed point is observed at three loops, consistently with Ref. 4. As the number l of loops increases, a fixed point—quite stable with respect to l—clearly appears. This is related to the appearance of a second upper branch of zeros of $\beta_{\overline{u}}(\overline{u},\overline{v})$. For N

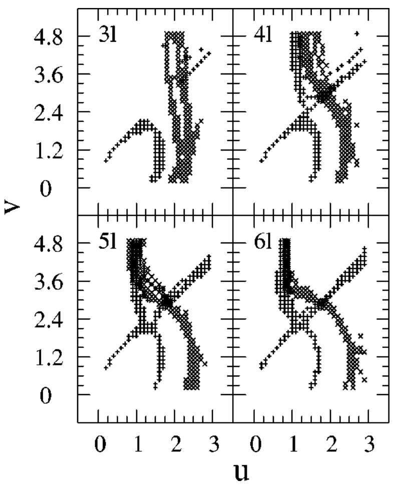

FIG. 2. Zeroes of the β functions for $N=3$ in the $(\bar{u},\bar{v})$ plane. Pluses $(+)$ and crosses $(\times)$ correspond to zeros of $\beta_{\bar{u}}(\bar{u},\bar{v})$ and $\beta_{\bar{v}}(\bar{u},\bar{v})$, respectively.

$=2$ (resp., $N=3$) such zeroes appear in 15, 45, 80, and 95 % (resp. 45, 70, 95, and 100 %) of the approximants we consider for $l=3,4,5,6$. Clearly, the set of zeros is increasingly stable as l increases. We obtain a fixed point for

$$\bar{u}^*=1.9(1), \qquad \bar{v}^*=4.10(15), \qquad \text{for} \quad N=2, \quad (4)$$

$$\bar{u}^*=1.8(1), \qquad \bar{v}^*=3.00(15), \qquad \text{for} \quad N=3, \quad (5)$$

where the error bars have been set quite conservatively: all zeros of the approximants with $3\leqslant b\leqslant 18$ and $0\leqslant\alpha\leqslant 4$ lie within the reported confidence interval. We stress again that for $l=6$ essentially all approximants show the presence of such fixed point. Its position is also stable with respect to the number of loops: an equivalent estimate is obtained for $l=5$. Notice that the fixed points belong to the region in which the series are not Borel summable, but still satisfy $\bar{v}^*/\bar{u}^*<4R_{2N}$. Thus, we expect our resummations to be reliable, and the stability of the results with respect to l confirms it.

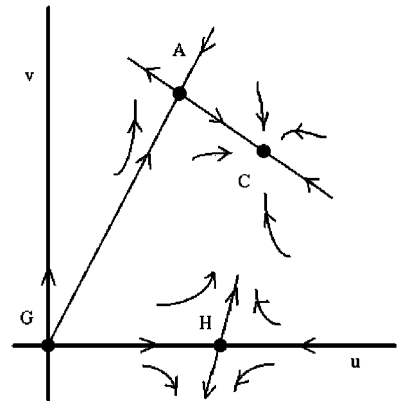

FIG. 3. RG flow in the (u,v) plane for $N=2,3$.

We then compute the eigenvalues of the stability matrix. They vary significantly with the two parameters α and b and turn out to be complex in most of the cases. Nonetheless, the sign of the real part of the eigenvalues is always positive, implying the stability of the fixed points. A reasonable estimate of the exponent ω is, however, impossible.

Figures 1 and 2 suggest also the presence of a second fixed point for smaller values of $\bar{u}$, say $\bar{u}\approx 1$, and thus, a RG flow diagram of the form reported in Fig. 3. Beside the stable chiral fixed point C, an additional unstable (antichiral) one A should be present. In our graphs, its position is rather imprecise, likely due to the fact that the relevant $\bar{u}$ and $\bar{v}$ belong to the region $\bar{v}/\bar{u}>4R_{2N}$, where resummation methods should be less effective.

Having established the existence of a stable fixed point, we compute the critical exponents from the corresponding six-loops series, following Ref. 13. The results are in substantial agreement with the experimental estimates, see Table I.

TABLE I. Critical exponents for $N=2$ and $N=3$. Our results are labeled by FT. Experimental results are reviewed, e.g., in Ref. 1.

N		γ	ν	β	α
2	$CsMnBr_3$	1.10(5) (Ref. 15)	0.57(3) (Ref. 15)	0.25(1) (Ref. 15)	0.39(9) (Ref. 16)
		1.01(8) (Ref. 17)	0.54(3) (Ref. 17)	0.22(2) (Ref. 17)	0.40(5) (Ref. 18)
				0.24(2) (Ref. 19)	
	$CsNiCl_3$			0.243(5) (Ref. 20)	0.37(8) (Ref. 21)
					0.342(5) (Ref. 22)
	$CsMnI_3$				0.34(6) (Ref. 21)
	FT	1.10(4)	0.57(3)	0.31(2)	0.29(9)
3	VCl_2	1.05(3) (Ref. 23)	0.62(5) (Ref. 23)	0.20(2) (Ref. 23)	
	VBr_2				0.30(5) (Ref. 24)
	$RbNiCl_3$			0.28(1) (Ref. 25)	
	$CsNiCl_3$			0.28(3) (Ref. 20)	0.25(8) (Ref. 21)
					0.23(4) (Ref. 22)
					0.28(6) (Ref. 26)
	FT	1.06(5)	0.55(3)	0.30(2)	0.35(9)

We also compare the six-loop results with the critical exponents that we computed to $O(1/N^2)$ in the framework of the large-N expansion. For example,

$$\nu = 1 - \frac{16}{\pi^2}\frac{1}{N} - \left(\frac{56}{\pi^2} - \frac{640}{3\pi^4}\right)\frac{1}{N^2} + O\left(\frac{1}{N^3}\right). \qquad (6)$$

We find $\nu = 0.858(4)$ for $N=16$ and $\nu = 0.936(2)$ for $N = 32$, which compare reasonably with the estimates that one obtains from Eq. (6), i.e., $\nu = 0.885$ for $N=16$ and $\nu = 0.946$ for $N=32$.

For $5 \lesssim N \lesssim 7$ the picture obtained from the analysis of the 6-loop series is less clear. We do not find fixed points that are sufficiently stable with respect to the number of loops. These results may be explained by the traditional picture in which there is a particular value of N, $N_c \approx 6$, such that for $N > N_c$ there is a stable fixed point smoothly related to the large-N and small-ϵ chiral fixed point. For $N < N_c$ a first-order transition is usually expected. However, our results for $N=2,3$ indicate that the situation is more complicated and that a second value $3 < N_{c2} < N_c$ may exist such that for $N < N_{c2}$ the system shows again a chiral critical behavior with a fixed point unrelated to the small-ϵ chiral fixed point.

In conclusion, the extension to six loops of the FT expansions solves the apparent contradictions between field theory and experiments. We find that different stable chiral fixed points exist for two- and three-component systems. The estimated exponents are in substantial agreement with experiments, whose conclusions on the nature of the phase transitions are thus confirmed. However, we note that first-order transitions are still possible for systems that are outside the attraction domain of the chiral fixed point. In this case, the RG flow runs away to a first-order transition. This may explain the Monte Carlo results of Ref. 7 where a first-order transition was clearly found for modified lattice systems.

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