The 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 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 new 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., Ref. \([1]\)). In spite of these efforts, the critical behavior of these systems is still unclear, 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. They may be modeled by using short-ranged Hamiltonians for \(N\)-component spin variables defined on a stacked triangular lattice as

\[
\mathcal{H}_{\text{STA}} = - J \sum_{\langle ij \rangle_{xy}} \vec{s}_i \cdot \vec{s}_j - J' \sum_{\langle ij \rangle_z} \vec{s}_i \cdot \vec{s}_j,
\]

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. 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 matrix-like 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., Ref. \([1]\)) are consistent with a second-order phase transition belonging to a new (chiral) universality class. This is partially supported by Monte Carlo simulations (see, e.g., Ref. \([1]\) and references therein). On the other hand, three-loop perturbative calculations at fixed dimension \(d = 3\) \([2]\) and within the framework of the \(\epsilon\)-expansion \([3]\) 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 \(N_c = 3.91\) \([2]\) and \(N_c = 3.39\) \([3]\).

To explain these contradictory results it has been suggested that these systems undergo weak first-order transitions, that effectively appear as second-order ones in numerical and experimental works. This hypothesis has been supported by studies based on approximate solutions of the Wilson RG equations \([1]\), and by Monte Carlo investigations \([6]\) of modified lattice spin systems which, according to general universality ideas, should belong to the same universality class of the Hamiltonian \([1]\), and which show a first-order transition.

For larger 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. \([1]\) 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. Of course, one may think that the observed disagreement is due to the shortness of the available series, thereby calling for an extension of the perturbative expansions to clarify the issue.

FT studies of systems with noncollinear order are based on the \(O(N) \times O(M)\) symmetric Hamiltonian \([7,10]\)

\[
\mathcal{H} = \int d^d x \left\{ \frac{1}{2} \sum_a \left[ (\partial_\mu \phi_a)^2 + r \phi_a^2 \right] + \frac{1}{4!} u_0 \left( \sum_a \phi_a^2 \right)^2 \right\}
\]
where \( \phi_a \) (1 \( \leq a \leq M \)) 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 [1].

For \( N = 2 \), which is the case relevant for frustrated two-component spin models, an \( \epsilon \)-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 [2], one can show that the \( XY \) fixed point is the only stable one \[\pi\] 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. However, it is still possible that other fixed points are present in the region \( v_0 > 0 \), although they are not predicted by the \( \epsilon \)-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 [3]. According to the three-loop analyses of Refs. [2,3], 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. [1] 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 new 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 \( \beta \)-functions \( \beta_u(u, v) \) and \( \beta_v(u, v) \). In the case of a continuous transition, when \( m \to 0 \), the couplings \( u, v \) are driven toward an infrared-stable zero \( u^*, v^* \) of the \( \beta \)-functions. On the other hand, the absence of stable fixed points is usually considered as an indication of a (weak) first-order transition.

In Tables 1 and 2 we present the six-loop expansion of the \( \beta \)-functions for \( M = 2 \), associated respectively with the rescaled couplings \( \tilde{u} = 3u/(16\pi R_{2N}) \) and \( \tilde{v} = 3v/(16\pi) \), where \( R_K \equiv 9/(8 + K) \). 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 \( \tilde{u} \) and \( \tilde{v} \) at fixed \( z = \tilde{v}/\tilde{u} \). For \( z \equiv \tilde{v}/\tilde{u} \) fixed and \( M = 2 \), the singularity of the Borel transform closest to the origin, \( \tilde{u}_b \), is given by

\[
\frac{1}{\tilde{u}_b} = -aR_{2N} \quad \text{for} \quad 4R_{2N} > z > 0, \tag{3}
\]

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

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. [10] to the analysis of the RG

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
\( t, j \) & \( \beta_u^{(t)} \) & \( \beta_v^{(t)} \) & \( R_{2N}^{t-1} \beta_i^{(t)} \) \\
\hline
2.0 & -2(N-1)/9 & 0.2 & -318.193529 & +0.00018978314 N^3 \\
3.1 & -895+31N/2187 & 2.1 & 400(N-1)/2187 & 1.2 & -118(N-1)/729 & 0.5 & 10(N-1)/243 \\
4.0 & 0.27365517 + 0.15072806 N + 0.007401604 N^2 & 3.1 & (N-1) (-0.22580775 - 0.0182536 N) & 2.2 & (N-1) (0.26899335 + 0.020914067 N) & 1.3 & (N-1) (-0.11448007 - 0.005283250 N) & 0.4 & (N-1) (0.009884444 - 0.001662474 N) \\
5.0 & -0.2927672 - 0.1856745 N + 0.000183529 N^2 & 4.1 & (N-1) (0.31461221 + 0.055501872 N - 0.00682480222 N^2) & 2.3 & (N-1) (0.2585304 + 0.37648759 N - 0.00012117624 N^2) & 1.4 & (N-1) (-0.059022058 + 0.0045733835 N + 0.007317786 N^2) & 0.5 & (N-1) (0.0068557471 - 0.0002180575 N - 0.00002544303 N^2) \\
6.0 & 0.35174477 + 0.26485903 N - 0.051288106 N^2 & 5.1 & (N-1) (-0.50696692 - 0.12967024 N - 0.001477485 N^2) & 2.4 & (N-1) (0.21149268 + 0.450557077 N - 0.0009000169 N^2) & 1.5 & (N-1) (-0.040302694 - 0.0003126947 N + 0.0000414932 N^2) & 0.6 & (N-1) (0.0021121351 + 0.0001368763 N + 0.000014729631 N^2) \\
7.0 & -0.5194089 - 0.4297650 N - 0.09535750 N^2 & 6.1 & (N-1) (0.000490135 N + 0.009022624 N^2 + 1.410456 \times 10^{-6} N^5) & 3.4 & (N-1) (-0.6451180 - 0.2271141 N - 0.007968847 N^2) & 1.6 & (N-1) (-0.02753284 - 0.009932742 N - 0.00004985576 N^2) & 0.7 & (N-1) (0.000298855 + 0.0003424570 N - 0.00005976447 N^2 + 3.644114 \times 10^{-6} N^0 - 1.527023 \times 10^{-6} N^0) \\
\hline
\end{tabular}
\caption{Coefficients \( \beta_i^{(t)} \) of the six-loop expansion of \( \beta_u \)}
\end{table}
functions of the cubic model. We resum the perturbative series by means of an appropriate conformal mapping that takes into account the large-order behavior of the perturbative series at fixed $\varepsilon$ and turns the original series into a convergent sequence of approximations. To understand the systematic errors we vary two different parameters, $b$ and $\alpha$, in the analysis. We apply this method also for those values of $\varepsilon$ 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 $\varepsilon < 4R_{2N}$, 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 $\beta$-functions, obtained from the analysis of the $l$-loop series, $l = 3, 4, 5, 6$. For each $\beta$-function we consider 18 different approximants with $b = 3, 6, \ldots, 18$ and $\alpha = 0, 2, 4$ and we determine the lines in the $(\bar{u}, \bar{v})$ plane on which they vanish. Then, we divide the domain $0 \leq \bar{u} \leq 4$ and $0 \leq \bar{v} \leq 5$ into $40^2$ rectangles, marking those in which at least two approximants of each $\beta$ function vanish. No fixed point is observed at three loops, 3
results are labelled by FT. Experimental and Monte Carlo

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

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 \( N = 32 \).

In conclusion, the extension to six loops of the FT expansions solves the apparent contradictions between field theory and experiments. We find that new 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.