

Chiral exponents in frustrated spin models with noncollinear order

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We compute the chiral critical exponents for the chiral transition in frustrated two- and three-component spin systems with noncollinear order, such as stacked triangular antiferromagnets (STA). For this purpose, we calculate and analyze the six-loop field-theoretical expansion of the renormalization-group function associated with the chiral operator. The results are in satisfactory agreement with those obtained in the recent experiment on the XY STA CsMnBr₃ reported by [V. P. Plakhty *et al.*, Phys. Rev. Lett. **85**, 3942 (2000)], providing further support for the continuous nature of the chiral transition.

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The critical behavior of frustrated spin systems with noncollinear order is still a controversial issue, field-theoretical (FT) methods, Monte Carlo (MC) simulations, and experiments providing contradictory results in many cases. At present there is no agreement on the nature of the phase transition, and in particular on the existence of a new chiral universality class.¹ See, e.g., Refs. 2–4 and Refs. 5–7 for reviews.

In 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 two- and three-component antiferromagnets on stacked triangular lattices.⁸ Their behavior at the chiral transition may be modeled by a short-ranged Hamiltonian for N -component spin variables $\vec{S} = \{S_i\}$, defined on a stacked triangular lattice as

$$\mathcal{H}_{\text{STA}} = -J \sum_{\langle vw \rangle_{xy}} \vec{S}(v) \cdot \vec{S}(w) - J' \sum_{\langle vw \rangle_z} \vec{S}(v) \cdot \vec{S}(w), \quad (1)$$

where $J < 0$, the first sum is over nearest-neighbor pairs within triangular layers, and the second one is over orthogonal interlayer nearest neighbors. Frustration due to the competition of interactions is realized in helimagnets.

In these models 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. At criticality one expects 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. In particular, the ground state of the XY systems shows the 120° structure of Fig. 1, and it is Z_2 chirally degenerate according to whether the noncollinear spin configuration is right- or left-handed. The chiral degrees of freedom are related to the local quantity¹

$$C_{ij} \propto \sum_{\langle vw \rangle \in \Delta} S_i(v) S_j(w) - S_j(w) S_i(v), \quad (2)$$

where the summation runs over the three bonds of the given triangle. The definition of C_{ij} can be straightforwardly generalized to the case of N -component spins.

Many experiments are consistent with a second-order phase transition belonging to a new (chiral) universality class (see, e.g., Refs. 5 and 6 for reviews). Further experimental evidence in favor of a chiral continuous transition has been recently reported in Ref. 2, showing the simultaneous occurrence of spin and chiral order in the XY stacked triangular antiferromagnet (STA) CsMnBr₃.

On the theoretical side the issue has been controversial. MC simulations^{9–15} (see Refs. 6 and 7 for reviews) have not been conclusive in setting the question. Simulations of STA's are consistent with continuous transitions, but with critical exponents that are not in a satisfactory quantitative agreement. In Ref. 11 the results for the XY STA are interpreted as an evidence for mean-field tricritical behavior. Moreover, MC investigations¹⁵ of special lattice spin systems, that should belong to the chiral universality class on the basis of their symmetry, show clearly a first-order transition.

In a recent paper³ the issue has been studied by a continuous renormalization-group (RG) approach (see also Refs. 16 and 17). The results favor a first-order transition, since no evidence of stable fixed points is found. According to this first-order transition picture, the apparent continuous critical phenomena observed in experiments are interpreted as first-order transitions, weak enough to effectively appear as second-order ones. Note, however, that the practical implementation of this method requires an approximation and/or truncations of the effective action. So these studies may not be conclusive.

FT studies of systems with noncollinear order are based on the Landau-Ginzburg-Wilson $O(N) \times O(2)$ -symmetric Hamiltonian^{1,6}

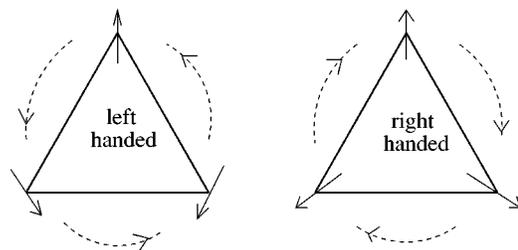


FIG. 1. The ground-state configuration of three XY spins on a triangle coupled antiferromagnetically.

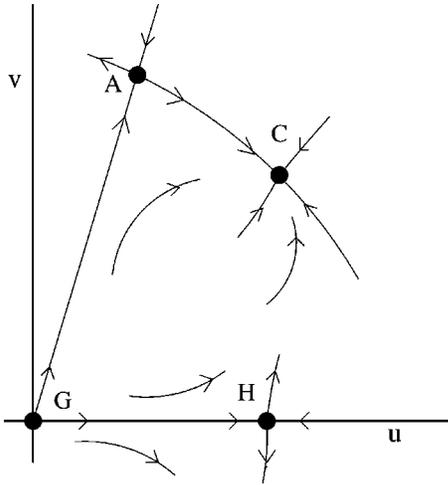


FIG. 2. RG flow in the quartic couplings (u, v) plane for $N = 2, 3$. It shows the stable chiral fixed point denoted by C , and the unstable antichiral (A), $O(2N)$ Heisenberg (H) and Gaussian (G) ones.

$$\mathcal{H} = \int d^3x \left\{ \frac{1}{2} \sum_a [(\partial_\mu \vec{\phi}_a)^2 + r \vec{\phi}_a^2] + \frac{1}{4!} u_0 \left(\sum_a \vec{\phi}_a^2 \right)^2 + \frac{1}{4!} v_0 \sum_{a,b} [(\vec{\phi}_a \cdot \vec{\phi}_b)^2 - \vec{\phi}_a^2 \vec{\phi}_b^2] \right\}, \quad (3)$$

where $\vec{\phi}_a = \{\phi_{ai}\}$, $1 \leq a \leq 2$ and $1 \leq i \leq N$, are two sets of N -component vectors. Frustrated XY and Heisenberg spin systems with noncollinear ordering, such as STA's, are described respectively by the $N=2$ and $N=3$ case with $v_0 > 0$. The presence of a stable chiral fixed point, conjectured by Kawamura,^{1,6} has been recently confirmed by the analysis of the perturbative six-loop series in the framework of the fixed-dimension expansion.^{4,18} As sketched in Fig. 2, a stable chiral fixed point C appears for both XY and Heisenberg cases. The critical exponents characterizing the stable chiral fixed point turn out to be in satisfactory agreement with experiments. Note that in this RG picture 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 some experiments (for example those for the CsCuCl_3 compound, see, e.g., Refs. 5 and 6) and MC studies for special lattice systems,¹⁵ where first-order transitions are observed.

Beside the conventional critical exponents β , γ , ν , etc., related to the standard spin order, one may consider additional critical exponents related to the behavior of the chiral degrees of freedom. If spin and chiral order occur simultaneously, one expects $\nu_c = \nu$ where ν_c is the exponent associated with the correlation length defined from the chiral correlation function. Introducing a chiral external field h_c coupled with the chirality C_{ab} , one may write the singular part of the free energy as¹

$$F_{\text{sing}} \propto t^{2-\alpha} f(h/t^\Delta, h_c/t^{\phi_c}), \quad (4)$$

where t is the reduced temperature, $\Delta = \beta + \gamma$, and ϕ_c is the chiral crossover exponent. Then, differentiating with respect to h_c , one may obtain the RG relations

$$\beta_c = 3\nu - \phi_c, \quad \gamma_c = 2\phi_c - 3\nu, \quad (5)$$

where the exponents β_c and γ_c describe respectively the critical behavior of the average chirality and of the chiral susceptibility.

Experimental estimates of the chiral exponents ϕ_c and β_c have been recently reported in Ref. 2 for the transition of the XY STA CsMnBr_3 :

$$\phi_c = 1.28(7), \quad \beta_c = 0.44(2), \quad (6)$$

measured respectively in the high- and low-temperature phase. On the theoretical side, there are a few MC results for the STA spin models (1), and very little from field-theoretical approaches. The chiral exponents have been only computed to $O(1/N)$ and $O(\epsilon)$ in the corresponding expansion frameworks.¹ However, these results do not allow a quantitative comparison, essentially for two reasons: because the series are too short and, most importantly, as discussed in Ref. 19, the chiral fixed point for the XY and Heisenberg cases is not analytically connected with the one found in the large- N and small- ϵ region. In order to obtain results that can be compared with experiments, one should compute them directly for $d=3$ and for the number of components of interest, i.e., $N=2, 3$.

In this paper we compute the chiral exponents using the fixed-dimension FT approach, by computing and analyzing the six-loop perturbative expansion of the chiral RG functions. In the fixed-dimension FT approach one performs an expansion in powers of appropriately defined zero-momentum quartic couplings (see, e.g., Ref. 7 and references therein). In order to obtain estimates of the universal critical quantities, the perturbative series are resummed and then evaluated at the fixed-point values of the couplings. The comparison with the experimental results (6) will represent a highly nontrivial check of the FT description of the transition and of the Kawamura's conjecture that these systems undergo continuous transitions belonging to distinct chiral universality classes.

In order to compute the universal quantities characterizing the critical behavior in the high-temperature phase, one introduces a set of zero-momentum conditions for the (one-particle irreducible) two-point and four-point correlation functions (see, e.g., Ref. 7 for details), which relate the zero-momentum quartic couplings u and v and the mass scale m to the corresponding Hamiltonian parameters u_0 , v_0 and r . In particular,

$$\Gamma_{ai,bj}^{(2)}(p) = \delta_{ab} \delta_{ij} Z_\phi^{-1} [m^2 + p^2 + O(p^4)]. \quad (7)$$

In addition, one defines the function Z_t through the relation $\Gamma_{ai,bj}^{(1,2)}(0) = \delta_{ab} \delta_{ij} Z_t^{-1}$, where $\Gamma^{(1,2)}$ is the (one-particle irreducible) two-point function with an insertion of $\frac{1}{2} \phi^2$. The fixed points of the theory are given by the common zeros u^* , v^* of the β functions

$$\beta_u(u,v) = m \frac{\partial u}{\partial m}, \quad \beta_v(u,v) = m \frac{\partial v}{\partial m}, \quad (8)$$

calculated keeping u_0 and v_0 fixed. The critical behavior is determined by the stable fixed point of the theory. The analysis of the six-loop expansion of the β -functions provides a rather robust evidence of the existence of a stable fixed point⁴ as shown in Fig. 2. The critical exponents η and ν are then derived by evaluating the RG functions

$$\eta_\phi(u,v) = \frac{\partial \ln Z_\phi}{\partial \ln m}, \quad \eta_t(u,v) = \frac{\partial \ln Z_t}{\partial \ln m} \quad (9)$$

at the chiral fixed point u^* , v^* . The resulting exponents are $\nu=0.57(3)$, $\eta=0.09(1)$, $\gamma=1.13(5)$ for the XY case, and $\nu=0.55(3)$, $\eta=0.10(1)$, $\gamma=1.06(5)$ for the Heisenberg case,²⁰ which are in substantial agreement with the experimental results.

In order to evaluate the chiral exponents, we consider the operator

$$C_{cd,kl}(x) = \phi_{ck}(x)\phi_{dl}(x) - \phi_{cl}(x)\phi_{dk}(x), \quad (10)$$

and define a related renormalization function Z_c from the one-particle irreducible two-point function $\Gamma^{(C,2)}$ with an insertion of the operator $C_{cd,kl}$, i.e.,

$$\Gamma^{(C,2)}(0)_{ai;bj;cd,kl} = Z_c^{-1} T_{abcd,ijkl}, \quad (11)$$

where

$$T_{abcd,ijkl} = (\delta_{ac}\delta_{bd} - \delta_{ad}\delta_{bc})(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}), \quad (12)$$

so that $Z_c(0,0) = 1$. Then, we compute the RG function

$$\eta_c(u,v) = \frac{\partial \ln Z_c}{\partial \ln m} = \beta_u \frac{\partial \ln Z_c}{\partial u} + \beta_v \frac{\partial \ln Z_c}{\partial v}, \quad (13)$$

and its value η_c at $u=u^*$, $v=v^*$, where u^* , v^* is the position of the stable chiral fixed point.⁴ Finally, the RG scaling relation

$$\phi_c = (2 + \eta_c - \eta)\nu \quad (14)$$

allows us to determine ϕ_c .

We computed $\Gamma^{(C,2)}(0)$ to six loops. The calculation is rather cumbersome, since it requires the evaluation of 563 Feynman diagrams. We handled it with a symbolic manipulation program, which generates the diagrams and computes the symmetry and group factors of each of them. We used the numerical results compiled in Ref. 21 for the integrals associated with each diagram. The resummation of the series was performed using the method outlined in Refs. 22 and 4. The

very lengthy expression of the six-loop expansion of $\eta_c(u,v)$, details of its calculation, and its analysis will be reported elsewhere.

The results of our analysis are

$$\phi_c = 1.43(4) \text{ for } XY, \quad (15)$$

$$\phi_c = 1.27(4) \text{ for Heisenberg.} \quad (16)$$

The errors are indicative of the spread of the results yielded by the analysis when changing the resummation parameters and varying the location of the chiral fixed point within the range reported in Ref. 4. Using the RG relations (5) and the estimates of ν ,⁴ one may also derive corresponding results for the other chiral exponents, obtaining for example

$$\beta_c = 0.28(10) \text{ for } XY, \quad (17)$$

$$\beta_c = 0.38(10) \text{ for Heisenberg.} \quad (18)$$

We may compare these results with the experimental ones (6). Our estimate of ϕ_c is somewhat higher than the estimate (6) while the estimate of β_c is correspondingly somewhat lower. In any case, the difference is of the order of one combined error bar. We may also compare our results to the available MC estimates²³ for the XY STA spin model, that are $\beta_c=0.45(2)$, $\gamma_c=0.77(5)$, $\phi_c=1.22(6)$ from Ref. 9, and $\beta_c=0.38(2)$, $\gamma_c=0.90(9)$, $\phi_c=1.28(10)$ from Ref. 11 (in this work a mean-field tricritical behavior is conjectured for the transition). These results are close to the experimental ones and thus show the same deviations with respect to our FT results.

For $N=3$ we can compare our results with the MC ones for the three-component STA spin model,²³ that are $\beta_c=0.55(4)$, $\gamma_c=0.72(8)$, $\phi_c=1.27(9)$ from Ref. 9 and $\beta_c=0.50(2)$, $\gamma_c=0.82(4)$ and $\phi_c=1.32(5)$ from Ref. 12. The FT estimate of ϕ_c is in perfect agreement with the MC results, while the estimate of β_c is somewhat lower, although compatible within error bars. Apparently, this is due to the fact that our estimate of ν is somewhat lower—but nonetheless in substantial agreement within error bars—than those obtained in MC simulations.

In conclusion, the FT results are in satisfactory agreement with the experimental and MC estimates. This is a nontrivial check of the FT approach, shows its predictive power in spite of the fact that the perturbative series are not Borel summable—still we take into account the leading diverging behavior, see Ref. 4—and strengthens the evidence for the continuous nature of the chiral transition in XY and Heisenberg STA's.

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⁸Examples of STA 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.

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