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Two-step transitions in noncollinear magnets

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A possibility for a two-step transition in noncollinear (twisted) magnets is studied by means of a renormalization-group (RG) technique near two dimensions. The microscopically derived RG equations allow a single transition governed by O(4) exponents but also two-step transitions with preliminary SO(2) or S_2 ordering, depending on the microscopical Hamiltonian. A possible experimental signature of partial ordering is discussed.

In the last few years there has been considerable interest in the study of frustrated antiferromagnets where a lattice type or a competition between couplings favors noncollinear spin ordering, which completely breaks down SO(3) symmetry. Well-known examples are helical magnets (Ho, Dy, Tb) where the spins are aligned ferromagnetically in a plane and form spirals in the perpendicular direction,[1] antiferromagnets on a stacked triangular lattice [$CsNiCl_3$,[2] $CsMnBr_3$,[3] VCl_2, VBr_2 (Ref. 4)] and on a body-centered-tetragonal lattice [$MnAu_2$, β-MnO_2 (Ref. 5)] and antiferromagnets on a Kagomé lattice [^{3}He adsorbed on graphite (Ref. 6), $SrCr_{7.13}Ga_{4.87}O_{19}$].[7]

There are two independent items which ensure an interest in the study of noncollinear spin systems. First is an apparent nonuniversality in the measured critical exponents for three-dimensional (3D) ordering transitions; these differ from each other significantly in different substances.[8] Moreover, perturbation expansion near four dimensions shows no stable fixed point in two orders in ϵ.[9] Two possible explanations involve a prediction of a new universality class associated with the relevance of a chirality operator[8] and a proposal[10] that all the systems under study are close to the tricritical point separating a first-order transition from a continuous one governed by the $n=4$ exponents.

On the other hand, a study of the magnetic properties of doped antiferromagnets in the context of high-T_c superconductivity focused attention on 2D square-lattice models with first-, second- (diagonal), and third-neighbor antiferromagnetic couplings (J_1-J_2-J_3 model).[11–13] This model is predicted to have a region of a disordered spin-liquid state even for large S, since quantum corrections, normally finite in 2D at zero temperature, diverge logarithmically on a second-order transition line $J_1=2J_2+4J_3$ between the antiferromagnetic (π,π) phase and noncommensurate phases [(Q,Q) or (π,Q) depending on the ratio of second- and third-neighbor couplings].[12] A conjecture made by Haldane,[14] that in the 2D case a paramagnetic phase with completely restored symmetry due to quantum fluctuations exists only for $2S=0$ (mod 4) while for the other S at least some discrete symmetry (presumably, a symmetry of translations by one site) must be broken, initiated an intensive study of a disordered state of this model with special attention to $S=\frac{1}{2}$.[11] Apart from a possible breakdown of a discrete symmetry, Chandra, Coleman, and Larkin[15] argued that the growth of noncommensurate SO(3) helical ordering may occur in two steps via an intermediate partly ordered state which resembles a P-type spin nematic[16] and has long-range order in a twist correlation function but no site magnetization in a plane perpendicular to the twist. More generally, the idea is that the twist and site magnetization—the constituents of the SO(3) order parameter—may decouple from each other.

In the present paper, I study the possibility for a decoupling by means of the now familiar RG technique near one dimension for zero-temperature transitions and near two dimensions for $T\neq 0$. The results of the ϵ expansion for *microscopical* Hamiltonians show that besides a single transition governed by O(4) exponents, two-step transitions with preliminary S_2 *or* SO_2 ordering are also possible. For definiteness, I will focus on a situation near two dimensions.

The standard approach to the stacked triangular antiferromagnet is based on a Landau-Ginzburg-Wilson effective action for noncollinear order parameter given by two vectors, $\mathbf{\Phi}_1$ and $\mathbf{\Phi}_2$.[17] This action obviously has SO(3)×SO(2) symmetry. In the ground state $\mathbf{\Phi}_1\cdot\mathbf{\Phi}_2=0$ and $\mathbf{\Phi}_1^2=\mathbf{\Phi}_2^2$ which implies that the system is invariant under SO(2) rotations. This subgroup of SO(3)×SO(2) is referred to as $SO(2)_{diag}$. The low-energy theory for $2+\epsilon$ expansion is then given by a nonlinear σ model on a coset space, $[SO(3)\times SO(2)]/SO(2)_{diag}$.[10] Once the order-parameter manifold is fixed, the action is expressed in a unique way in terms of the SO(3) rotation matrix R,

$$S=\frac{1}{2}\int d^dx\,\mathrm{Tr}[P(R^{-1}\nabla_\mu R)^2]\,,\quad P=\mathrm{diag}(g_1,g_1,g_2)\,. \tag{1}$$

It is convenient to rewrite this action through three Euler angles which parametrize SO(3) rotations

$$S=g_1(\nabla_\mu\varphi+\cos\theta\nabla_\mu\psi)^2+\frac{1}{2}(g_1+g_2)[(\nabla_\mu\theta)^2+\sin^2\theta(\nabla_\mu\psi)^2]\,. \tag{2}$$

As is clearly seen from (2), a nonlinear σ model on a coset space describes fluctuations of a unit vector [second term in (2)] combined in a particular way dictated by the symmetry manifold $[SO(3)\times SO(2)]/SO(2)_{diag}$ with the fluctuations of a scalar field φ.

One way to obtain RG equations near two dimensions, which I will follow by the purposes clarified below, is to bosonize Eq. (2) assuming the initial ordering with $\theta=\pi/2$. This procedure reduces Eq. (2) to a system of three initially Goldstone bosons with quadric anharmonisms, which come from the $\tilde{\theta}^2(\nabla_\mu\psi)^2$ term in (2) ($\tilde{\theta}=\pi/2-\theta$) and describe interactions between the constituents of the vector part of the order parameter, and cubic anharmonisms, which are produced by $\tilde{\theta}\nabla_\mu\psi\nabla_\mu\varphi$ and describe the interactions between vector and scalar parts of the order parameter. The coupling constants measuring the strength of these fluctuations are

$$g_A=\frac{g_2-g_1}{(g_1+g_2)^2},\quad g_B=\frac{g_1}{(g_1+g_2)^2}, \tag{3}$$

respectively. The RG equations are obtained in the same manner as for bipartite antiferromagnets.[18] Up to first order in ϵ they read

$$\dot{g}_B=g_B^2+2g_Ag_B-\epsilon g_B\,,\quad \dot{g}_A=g_A^2-g_Ag_B-\epsilon g_A\,. \tag{4}$$

These equations were obtained by Friedan[19] and applied to triangular antiferromagnets by Azaria, Delamotte, and Jolicoeur.[10]

Apart from a trivial fixed point, $g_A=g_B=0$, Eqs. (4) produce three nontrivial fixed points (Fig. 1). One of them, $g_A=2\epsilon/3$, $g_B=-\epsilon/3$, though stable, is only suggestive in a gradient approach since it corresponds to negative g_1. The remaining two are $g_A=0$, $g_B=\epsilon$ (point A) and $g_B=0$, $g_A=\epsilon$ (point B). Point A is a stable fixed point (i.e., it has only one direction of instability). It corresponds to $g_1=g_2$ and describes an ordinary second-order transition with O(4) critical exponents, when the symmetry breaks simultaneously for both the vector and scalar constituents of the SO(3) order parameter, which become indistinguishable at $g_1=g_2$. On the other hand, point B corresponds to $g_1=0$, i.e., to a decoupling between S_2 and SO(2) fluctuations. However, this fixed point is unstable (both eigenfrequencies are equal to ϵ) and has no basin of attraction. It thus follows that a description of noncollinear magnets in terms of a nonlinear σ model on a coset space violates any possibility for a two-step transition through a partly ordered phase.

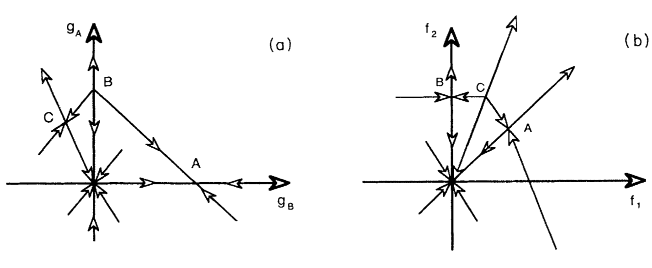

FIG. 1. Renormalization-group flows governed by the RG equations (4) and (5) [Figs. (a) and (b), respectively]. In both cases, RG equations produce a stable fixed point A, which describes a single second-order transition governed by O(4) exponents. However, a fixed point B at $g_B(f_1)=0$, which corresponds to a decoupling between S_2 and SO(2) fluctuations, is unstable within a rotation matrix approach, but has a finite basin of attraction for microscopically derived RG equations.

In principle, Eq. (1) can be derived for any particular Hamiltonian of a noncollinear magnet by expressing the site spin as $\mathbf{S}(\mathbf{r})=R(\mathbf{r})\mathbf{S}_0(\mathbf{r})$, where $\mathbf{S}_0(\mathbf{r})$ is a classical spin configuration. This was done by Dombre and Read[20] for triangular antiferromagnets with nearest-neighbor Heisenberg coupling J. For bare couplings, they obtained

$$g_B^0=-g_A^0=(4/\sqrt{3})(T/JS^2)\,.$$

The same procedure applied to J_1-J_2-J_3 model yields for $J_2=0$,

$$g_B^0=-g_A^0=\left(\frac{T}{2J_3S^2}\right)\left(\frac{16J_3^2}{16J_3^2-J_1^2}\right)$$

(helical ordering is present when $4J_3>|J_1|$).

Contrary to the results of a macroscopic approach, Chandra and Coleman[21] argued that, in a real quantum spiral structure, fluctuations of the twist director and of the on-site magnetization are quite different from each other, and, in particular, the slow rotations of the twist director are described not by conventional spin waves, which were predicted to acquire a finite gap at the corresponding momenta $k=\pm(Q,Q)$, but by longitudinal collective modes. From the symmetry point of view, this separation of the fluctuations of the twist director and of on-site magnetization, if it actually exists, would imply that the fluctuating fields are defined on a manifold $S_2\times SO(2)$ rather than on a coset space $[SO(3)\times SO(2)]/SO(2)_{\rm diag}$. In this case, there are no reasons to expect that O(4) fixed point will survive as the only stable fixed point in $2+\epsilon$ expansion.

To resolve this contradiction, I considered low-energy fluctuations in both, triangular antiferromagnets and J_1-J_2-J_3 model in the frameworks of a direct $1/S$ expansion, i.e., without appealing to any particular choice of the order-parameter manifold. For simplicity, in case of the J_1-J_2-J_3 model I restricted with the (Q,Q) helical ordering and set $J_2=0$. I did not find a breakdown of a spin-wave description when quantum fluctuations are present in the system, but *microscopically* derived RG equations surprisingly turned out to be different from those obtained in a σ-model formalism.

The calculations were performed in a standard manner by using a bosonization procedure based on a Dyson-Maleev transformation.[18] After diagonalization, the quadratic in bosons part of the Hamiltonian obviously describes noninteracting transverse spin waves with the spectrum which has three Goldstone modes at $k=0$ and $k=\pm(Q,Q)$, where $Q=2\pi/3$ for triangular antiferromagnets and $\cos Q=-J_1/4J_3$ for the J_1-J_3 model.[22] The $k=\pm(Q,Q)$ zero modes result from fixing of a direction of a twist while $k=0$ zero mode reflects a breakdown of a rotational symmetry in a plane perpendicular to a twist. Higher-order terms in bosonic operators give rise to the interactions between spin waves. For $2+\epsilon$ expansion, one should restrict to the low-energy fluctuations near soft modes and calculate logarithmical renormalization of the vertex functions.

In principle, the theory contains both cubic and quartic vertices. However, I have checked that cubic vertices do not undergo logarithmical renormalization and thus play no role in the perturbative expansion near two dimensions. At the same time, the coupling constants measuring the strength of quartic interactions flow in passing to larger scales.

There are two types of fourfold anharmonic terms. The first, with a coupling f_1, describes interactions between soft modes near $k=\pm(Q,Q)$ and near $k=0$ (i.e., between vector and scalar parts of the order parameter), while the second, with a coupling f_2, describes interactions between soft modes at $k=\pm(Q,Q)$, i.e., between the constituents of the vector part of the order parameter.[23] This term is exactly the same as in the bosonized version of Eq. (2). Moreover, the bare couplings f_1^0 and f_2^0 *exactly* coincide with g_B^0 and g_A^0, correspondingly. The calculation of f_2^0 requires special care since if we restrict with only fourfold terms, then the vertex function for $\pm(Q,Q)$ interaction will not fit the Adler principle and immediately will give rise to a gap $\Delta\sim\sqrt{S}$ at $\pm(Q,Q)$ in the spin-wave spectra.[21] However, this fourfold interaction is strongly renormalized by the second-order perturbation contribution from cubic terms with the momenta of the intermediate boson around $2Q$.[24] This contribution recovers a correct structure of the fourfold vertex and, hence, zero modes at $\pm(Q,Q)$ in the spin-wave spectra.[24,25] Note that the cubic terms with one of the momenta around $2Q$ represent contributions from the gap modes and should not be confused with the cubic terms describing the interactions between soft modes with k near 0 and (Q,Q), which were proved to be unimportant near two dimensions.

While the fluctuations within the vector part of the order parameter are described by exactly the same bosonic Hamiltonian in both the σ model and spin-wave approaches, the interactions between the vector and scalar parts of the order parameter are produced by different anharmonic terms: by cubic anharmonisms in the σ-model description and by quartic anharmonisms in the nonlinear spin-wave theory. As a consequence, the RG equations, obtained microscopically, differ from those of Eqs. (4), and in the two-loop approximation read

$$\begin{aligned}\dot{f}_1&=f_1(1+f_1)(f_1+f_2)-\epsilon f_1\,,\\ \dot{f}_2&=f_1^2(1+f_1)+f_2^2(1+f_2)-\epsilon f_2\,.\end{aligned}\tag{5}$$

In agreement with the results of a σ-model approach, Eqs. (5) also have a stable fixed point A with $f_1^{(c)}=f_2^{(c)}=\epsilon/2(1-\epsilon/2)$,[26] which represents an ordinary second-order transition with O(4) exponents, when the symmetry breaks simultaneously for both parts of the order parameter. However, the remaining two nontrivial fixed points of Eqs. (5) differ from those of Eqs. (4) and coincide with each other within a one-loop approximation, so that one has to go to a two-loop order to distinguish between them. It then follows from (5) that the O(3) fixed point with $f_1^{(c)}=0$, $f_2^{(c)}=\epsilon(1-\epsilon)$ (point B) is *stable,* i.e., has a finite basin of attraction. The third fixed point (point C) has $f_1^{(c)}=\epsilon^2$, $f_2^{(c)}=\epsilon\;(1-\epsilon)$ and is unstable. The renormalization-group flows in the (f_1,f_2) plane for small ϵ are presented in Fig. 1(b).

Formally, the bare couplings f_1^0 and f_2^0, found in a semiclassical approximation, are in a basin of attraction of the O(4) fixed point A. In this sense, rotation matrix and spin-wave approaches describe the same physics. However, the ratio of the couplings is a nonuniversal quantity and may change due to short-range quantum corrections or in more complicated models. In view of this, it seems useful to also discuss a more intriguing possibility allowed by the RG equations of Eq. (5). Specifically, in dimensions higher than two a *finite* positive attraction between bosonic fields describing the fluctuations of vector and scalar parts of the order parameter (i.e., finite positive $f_1^{(0)}$) is necessary to produce O(4) behavior. For small enough $f_1^{(0)}$, the RG equations drive the system to the other stable fixed point B with $f_1^{(c)}=0$. In this case the fluctuations of vector and scalar parts of the order-parameter *decouple* at large scales and for $f_2>f_2^{(c)}$ only S_2 fluctuations acquire a gap, while SO(2) fluctuations remain gapless up to a much higher temperature of Berezinskii-Kosterlitz-Thouless transition.[27] In the intermediate phase there is no long-range magnetic order, nor chirality, but there is a gapless branch of excitations and some correlations decay by a power law. For example, in triangular antiferromagnets this would be the case for out-of-plane fluctuations of a total spin of a triad which are expressed solely in terms of $k\approx 0$ bosons.[28]

In principle, Eqs. (5) also allow a second possibility. The point is that for nonzero ϵ, while scaling over a temperature along $f_2^{(0)}=-\eta f_1^{(0)}$ with, in a general case, arbitrary η, one has a chance not to cross a separatrix driving the system to the O(4) fixed point. In the one-loop approximation, this separatrix starts near A as $f_2=-2f_1+(3\epsilon/2)$. Numerical and analytical calculations show that for large $f_{1,2}$ (on a scale of ϵ) it continues as $f_2=-\lambda f_1$, where $\lambda\approx 4.56$. Hence, for large enough η, the bare couplings will remain in a basin of attraction of the trivial fixed point independently on the temperature. Assuming that this remains true up to $T\sim J$, I come to a possibility, though suggestive, of a preliminary transition governed solely by the f_3 coupling, measuring the strength of SO(2) fluctuations. This is a realization of a conjecture made by Chandra, Coleman, and Larkin[15] that long-range order in a twist correlation function may survive a loss of in-plane magnetic ordering. The intermediate phase will have zero on-site magnetization and a gap for $k=0$ excitations but will keep a spontaneous symmetry breaking with respect to a twist (pseudo)vector and, hence, Goldstone modes at $k=\pm(Q,Q)$. This ordering does not break time-reversal symmetry and by this reason the intermediate phase is referred to as a P-type spin nematic.[15,16]

To summarize, it follows from the perturbative expansion near two dimensions that a continuous transition governed by O(4) exponents is a most probable, but not the only possibility for noncollinear antiferromagnets. The microscopically derived RG equations also allow two-step transitions with both the O(3) and O(2) preliminary ordering. The type of transition depends on the values of microscopic couplings.

Of course, $2+\epsilon$ expansion does not necessarily completely reproduce the situation in three dimensions. In particular, for sufficiently large ϵ two-step continuous transition may be substituted by a single first-order transition (which, evidently, cannot be detected within $2+\epsilon$ expansion). This is a typical situation for many orientational phase transitions.[29] In this, the present approach complements the hypothesis of Azaria, Delamotte, and Jolicoeur[10] that noncollinear antiferromagnets can undergo a first-order transition or a second-order one with O(4) or tricritical (classical) exponents depending on their microscopical Hamiltonians. Note also that as in Ref. 10, no "chiral" fixed point[8] was detected in the expansion near two dimensions.

Experimentally, the situation with 3D transitions is far from conclusive. The critical behavior with O(4) β exponent ($\beta=0.39$) was found in neutron-scattering experiments with rare-earth helimagnets Ho and Dy.[30] The other exponents, however, differ significantly from the O(4) ones.[31] On the other hand, Monte Carlo simulations[32] and experimental results[3] for $CsMnBr_3$ point out that triangular antiferromagnets undergo a transition with nearly classical exponents and thus are likely to be close to a tricritical point.[10] To my knowledge, no experiments point to the existence of two-step transitions in nearly isotropic 3D substances.[33] However, there is experimental evidence that the ground state in some quasi-2D substances may be partly ordered: Experiments with the Kagomé-lattice antiferromagnet $SrCr_{7.13}Ga_{4.84}O_{19}$ (Ref. 7) show that below $T=8$ K, the excitation spectrum is likely to be gapless [a specific heat, $C(T)\propto T^2$], while the two-spin correlation length is only twice the inter-Cr-atom spacing. As a possible explanation, one may assume that the orientational SO(2) ordering survives a loss of 120° magnetic ordering.[34] Whether this is indeed the case requires further investigation.

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