Second order phase transitions induced by disorder in frustrated magnets

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We study the critical properties of three dimensional frustrated magnets, diluted with non-magnetic impurities. We show that these systems exhibit a second order phase transition, corresponding to a new universality class. In the pure case, the phase transition is expected to be weakly of first order. We therefore argue that these frustrated systems can be used to study experimentally the rounding effect of disorder on discontinuous phase transitions. We give first estimates of the critical exponents associated with this universality class, by using the method of the effective average action.

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The influence of disorder on the properties of a system around a phase transition has triggered a lot of studies in the last twenty years. In the case of second order phase transitions, we have a fairly good understanding of the situation thanks to the Harris criterion [1, 2], which states that for a broad class of systems with quenched disorder, the critical exponent \( \nu \) (describing the singularity of the correlation length at the phase transition) must satisfy the inequality: \( \nu \geq 2/d \). This has a dramatic consequence for these pure materials for which the preceding inequality is not satisfied, since a small amount of disorder changes the critical exponents, such that the preceding inequality is fulfilled. The pure system is therefore unstable with respect to the inclusion of impurities, and one can expect a new universality class associated with the disordered system.

Although much less studied, the influence of disorder on materials undergoing first order phase transitions is also of great interest. In such a situation, the general trend is that quenched disorder smoothens the phase transition. In particular, Aizenman and Wehr [3] have proven that when disorder is coupled to a system of small enough dimensionality [4], the density conjugated to the disorder is a continuous function of the external parameters (temperature, magnetic field, etc.). For a system with random bonds (i.e. a random distribution of the interaction between nearest neighbors degrees of freedom), this statement implies that the energy density, which is then the density conjugated to the disorder, is a continuous function of the temperature. As a consequence, the latent heat vanishes: the transition is indeed smoothened by the disorder.

This rounding effect of the disorder has been also studied in specific models, mainly the random bond \( q \)-states Potts model. In two dimensions, Monte-Carlo simulations, as well as theoretical work show that the first order phase transition observed in the pure system for \( q \geq 5 \) becomes of second order when quenched disorder is introduced (see [4] and references therein). Monte-Carlo simulations on the three dimensional 3-states Potts model [5] display the same feature. However a shortcoming of the random bond Potts model for studying the rounding effect of the disorder, is that it seems difficult to find experimental realizations in the relevant cases. Indeed, for three-dimensional realizations of the Potts model, the disorder usually induces a random field term, and thus the relevant model is not the random bond Potts model [6]. On the other hand, in \( d = 2 \), it is required to find an experimental realization of the Potts model with at least five states, which seems quite difficult.

While studying the rounding effect of the disorder, it would be valuable to find an experimental realization of this situation. With this goal in mind, we consider in this letter the influence of non-magnetic impurities in \( XY \) and Heisenberg stacked triangular antiferromagnets (STA), such as CsMnBr\textsubscript{3}, CsNiCl\textsubscript{3}, and rare earth helimagnets (Ho, Tb, Dy). The spin degrees of freedom of these magnetic materials are submitted to competing interactions, which make the ground state more degenerate than in a non-frustrated system. For the pure case, it was soon proposed that a new universality class should be associated with the phase transition observed in these materials [6]; and from then on, there has been numerous works aimed at characterizing it. We have now strong evidences that this phase transition is actually weakly of first order, and not continuous as was initially proposed. Let us indicate the most striking evidences for this behavior in the \( XY \) case. First, most experimental and numerical studies indicate power-law behaviors of the physical observables around the transition temperature, characterized by a set of critical exponents. A detailed analysis shows that these critical exponents are most probably not compatible with those expected in a second order phase transition [7]. It is more likely that the phase transition is actually of first order, with such a large correlation length that the discontinuity at the phase transition cannot be observed in experiments. This scenario is confirmed by a recent Monte-Carlo simulation [8] in which a first order phase transition was directly observed, but only for very large lattice sizes. Finally, a renormalization-group calculation in the framework of the effective average action shows a lack of a stable fixed point [9] for both \( XY \) and Heisenberg cases, which in turn indicates that the phase transition is of first order. Note however that six-
loop resummed series indicate a true second order phase transition \[1\].

At the light of the introductory discussion, we propose to study the influence of quenched non-magnetic impurities in the critical behavior of STA and helimagnets. In particular, we want to show that in presence of impurities, the phase transition becomes continuous. We also want to characterize the associated universality class by giving a first estimate of the critical exponents. But before embarking on this discussion, let us stress on two evidences which indicate the importance of disorder in these systems. The first observation is that, in the pure case, the effective exponent \(\nu\) (0.54 < \(\nu\) < 0.57 \[12\]) is found to be much smaller than the lower bound 2/3 given by the Harris criterion (\(\nu < 2/d\) for disordered systems), so that we can expect the disorder to be strongly relevant. This conclusion is however an indication rather than a proof since Harris criterion only applies to second order phase transitions, which is not the case here. Second, the instability of the critical properties of the system when impurities are added has been tested experimentally on STA with diluted non-magnetic impurities \[13\], which shows, using scaling relation, that the exponent \(\nu\) increases strongly when impurities are introduced.

We now derive the action relevant for the materials under study. Let us consider the general situation of a diluted system of spins on a lattice, submitted to a two-body interaction, in vanishing magnetic field. The corresponding Hamiltonian reads:

\[
H = -\frac{1}{2} \sum_{i,j} J_{i,j} \epsilon_i \epsilon_j \vec{S}_i \cdot \vec{S}_j. \tag{1}
\]

Here, \(J_{i,j}\) represents the (translation invariant) interaction between spins at lattice sites \(i\) and \(j\), and the spins \(\vec{S}_i\) are \(n\)-component vectors normed to unity. In physical realizations of STA and helimagnets, the number of spin components is taken to be two or three, depending on the anisotropies of the material. The dilution appears through the random variables \(\epsilon_i\), which equal 0 if a non-magnetic impurity lies on site \(i\), and 1 otherwise. The \(\epsilon_i\) are chosen to be independent random variables with no dynamics, so as to describe a situation where the impurities are quenched. The associated partition function reads:

\[
Z = \int D\vec{S} \exp \left( -H \right). \tag{2}
\]

To deal with the unit norm constraint of \(\vec{S}_i\), we perform the standard Hubbard-Stratonovitch transform (we follow the discussion of \[14\]) and introduce the auxiliary field \(\vec{\psi}\), so that the partition function reads:

\[
Z = \int D\vec{S} D\vec{\psi} \exp \left( -\frac{1}{2} \sum_{i,j} J_{i,j}^{-1} \vec{\psi}_i \cdot \vec{\psi}_j - \sum_i \epsilon_i G_n(\vec{\psi}_i) \right) \tag{3}
\]

The variables \(\vec{S}_i\) at different lattice sites are now decoupled, and the integral on \(\vec{S}\) can be performed. One gets, up to an irrelevant multiplicative constant:

\[
Z = \int D\vec{\varphi} \exp \left( -\frac{1}{2} \sum_{i,j} J_{i,j}^{-1} \vec{\varphi}_i \cdot \vec{\varphi}_j - \sum_i \epsilon_i G_n(\vec{\varphi}_i) \right) \tag{4}
\]

where \[20\]:

\[
G_n(x) = -\ln \left( \frac{\int d^n y \delta(y^2 - 1) \exp(\vec{x} \cdot \vec{y})}{\int d^n y \delta(y^2 - 1)} \right), \tag{5}
\]

For deriving Eq.(4) we used the fact that the \(\epsilon_i\) take values in \{0, 1\}. In terms of the local magnetization \(\vec{\varphi}_i = \sum_j J_{i,j}^{-1} \vec{\varphi}_j\) \[14\], the partition function reads:

\[
Z = \int D\vec{\varphi} \exp \left( -\frac{1}{2} \sum_{i,j} J_{i,j} \vec{\varphi}_i \cdot \vec{\varphi}_j - \sum_i \epsilon_i G_n(\sum_j J_{i,j} \vec{\varphi}_j) \right) \tag{6}
\]

The important point here is that \(G_n(\vec{x})\) is a scalar under rotations (see Eq. \[5\]) and therefore depends only on \(\vec{x}^2\). We conclude that the disorder \(\epsilon_i\) couples to the microscopic field \(\vec{\varphi}\) through terms with even powers of \(\vec{\varphi}\) such as, for instance, the random mass term \(\epsilon_i \vec{\varphi}_i^2\), but not through terms linear in the field, which would correspond to the more complex situation of a random field.

We now specialize to the case of helimagnets and STA. In these materials, the spin degrees of freedom are submitted to competing interactions, which induce frustration. As a consequence, there are two critical modes \(\vec{\varphi}_\pm \vec{Q}\) (i.e. modes minimizing the two-point interaction \(J(\vec{q})\) in Fourier space), with \(\vec{Q}\) some characteristic momentum \[15\], instead of only one critical mode \(\vec{\varphi}_\vec{q}=0\) in the ferromagnetic case. In the long distance limit, the physics is governed by those modes whose momenta are very close to \(\pm \vec{Q}\), while the other modes only influence non-universal quantities, and can be discarded. We are therefore left to introduce two types of fields:

\[
\varphi_\pm(\vec{q}) = \varphi(\pm \vec{Q} + \vec{q}). \tag{7}
\]

It is convenient to perform the change of variables:

\[
\varphi_1(q) = \varphi_+(q) + i\varphi_-(q) \quad \varphi_2(q) = \varphi_+(q) - i\varphi_-(q) \tag{8}
\]

If we now expand the interaction potential \(G_n\) to fourth order in the fields, the partition function can be recast into the form:

\[
Z = \int D\vec{\varphi}_1 D\vec{\varphi}_2 \exp(-\mathcal{S}) \tag{9}
\]

with:

\[
\mathcal{S} = \int d^4 x \left\{ \frac{Z(x)}{2} \text{Tr} (\partial^4 \phi \partial^4 \phi) + \frac{\rho^4(x)}{2} + \frac{g_1(x)}{8} \rho^2 + \frac{g_2(x)}{4} \rho^2 \right\}, \tag{10}
\]
We have merged here the two n-components vectors \( \vec{\phi}_1 \) and \( \vec{\phi}_2 \) into a \( 2 \times n \) matrix \( \phi = (\vec{\phi}_1, \vec{\phi}_2) \), and introduced \( \rho = \text{Tr} (\rho \phi \phi^*) = \text{Tr} (\rho \phi^* \phi) \). This action is very similar to the one obtained in the pure case \([6, 7]\), except for the \( x \)-dependence of the field normalization \( Z \) and of the coupling constants \( r, g_1 \) and \( g_2 \), appearing through the presence of impurities (noted \( \epsilon_i \) in Eq. [6]). In the following, we consider a direct generalization of this situation where \( \phi \) is a \( m \times n \) matrix. For \( m = 2 \), we retrieve the case of physical interest discussed previously.

Once the action \([10]\) is determined, one would have to compute the quantity of interest for a given realization of the disorder (for a particular choice of the \( \{\epsilon_i\} \)). This is however a formidable task. A simpler strategy consists in using the previous action, and taking the limit \( \epsilon_i \to 0 \). \( \Gamma_k \) is then obtained by integrating over the \( \{\epsilon_i\} \), which interpolates smoothly between the microscopic action \( S \) (when \( k \to \infty \)) and the Gibbs free energy \( \Gamma \) (when \( k \to 0 \)). \( \Gamma_k \) therefore connects smoothly the macroscopic and microscopic descriptions of the system. For intermediate values of \( k \), \( \Gamma_k \) is obtained by integrating over the high momentum modes only, while long distance modes are effectively left unintegrated. A major interest of \( \Gamma_k \) is that its evolution with the scale \( k \) is governed by an exact, concise equation \([17]\):

\[
\frac{\partial \Gamma_k}{\partial t} = \frac{1}{2} \int_q \frac{\partial \Gamma_{k}(q)}{\partial \Gamma^{(2)}(q)} \cdot \left[ R_k(q) + R_k(q) \right],
\]

with \( k \propto \exp(t) \). The function \( R_k(q) \) describes how the low and high momentum modes are separated, and \( \Gamma^{(2)}_k \) is the second functional derivative of the effective average action. Although this equation cannot be solved exactly, it can be used in practice to determine nonperturbative flow equations. The idea consists in considering a truncation for \( \Gamma_k \), typically characterized by a finite number of coupling constants. By introducing this truncation in equation \([13]\), one deduces flow equations for the different coupling constants. These are non-polynomial in coupling constants, as can be seen from the nonlinear structure of the flow equation \([13]\).

We now describe the type of truncations considered here:

\[
\Gamma_k = \int_Z \frac{Z}{2} \sum_i \text{Tr} (\partial^\rho \phi_i \partial \phi_i) + \frac{u_1}{8} \sum_i (\rho_i - \kappa)^2 + \frac{u_2}{4} \sum_i (\tau_i - 2 \rho_i \kappa) + \frac{u_3}{8} \left( \sum_i (\rho_i - \kappa)^2 \right)^2
\]

This truncation is to be seen as the first terms of an expansion of the effective average action around a configuration \( \phi_{\text{stat}} \), defined by \( \langle \phi_{\text{stat}} \rangle = \sqrt{\rho} \delta_{ij} \) (here, \( i \) and \( j \), running respectively from \( 1 \) to \( n \) and from \( 1 \) to \( m \), stand for the matrix indices of the field, while \( l \) stands for the replica index, running from \( 1 \) to \( o \)). We have also considered truncations with \( \phi^6 \) terms added. The action depends then on six more coupling constants. The flow equations have been derived using the method presented above. However those are to lengthy to be displayed here. We only quote the flow equation in the limit of small coupling constants \( \{u_1, u_2, u_3\} \), which identify with the one loop expansion in coupling constant \([21]\):

\[
u_1 = -4u_1 + 2v_4 \left( (8 + mn)u_1^2 + 12u_2^2 + 4u_3 \right)
\]

\[
u_2 = -4u_2 + 2v_4 u_3 \left( (8 + mn)u_1^2 + 4u_3 \right)
\]

\[
u_3 = -4u_3 + 2v_4 u_3 \left( (8 + mn)u_1^2 + 4u_3 \right)
\]

where \( \varepsilon = 4 - d \), \( v_4 = 1/32\pi^2 \), and the dot indicates a derivative with respect to \( t \). For generic values of \( m \), \( n \) and \( \alpha \), the flow equations admit eight fixed points. Out of them, six are already well known. There are four fixed points with \( u_2 = 0 \), corresponding to the situation of a diluted system of \( mn \) components spins \([13]\), and two extra fixed points with \( u_3 = 0 \), corresponding to the pure
frustrated magnets. In addition, there are two new fixed points. We finally indicate that for certain values of \((m, n, o)\), there is a degeneracy of the one loop \(\beta\) functions (for example, for \(m = 2, o = 0, n \simeq 25.3\)). For such values of \((m, n, o)\), we expect a \(\sqrt{\varepsilon}\)-epsilon fixed point to appear at two-loop order, as in the random bond Ising model. We postpone the discussion of this point, as well as a more detailed description of the fixed points to a forthcoming publication.

In three dimensions, we have looked for roots of the \(\beta\) functions. In the case of physical interest \(m = 2\), the disorder is found to be irrelevant for \(n \gtrsim 5.5\). On the other hand, for \(n \lesssim 5.5\), the disordered fixed point is stable and governs the phase transition. We give on Fig.1 the values of the associated critical exponents. We first remark that our values of \(\nu\) are all smaller than the lower bound \(2/3\) predicted by the Harris criterion. However, for \(3 \leq n \leq 5.5\), \(\nu\) is off by only few percents, which is typically the error expected with the truncation considered here. The much larger discrepancy for \(n = 2\) can be attributed to the unusually large value of the anomalous dimension \(\eta\). In this case, richer truncations are to be considered in order to get more accurate results (work in progress). Although the accuracy of our results is questionable, in particular for \(n < 3\), they indicate that \(\nu\) is varying very slowly with \(n\) (in the pure vectorial model, the variation of \(\nu\) on the same range of \(n\) is almost ten times bigger), and that \(\nu\) is close to the lower bound \(2/3\) imposed by Harris criterion. These features are similar to what is observed in \(d = 2\) \(q\)-state Potts model with random bond using Monte-Carlo simulations, where \(\nu\) is found to be very close to the lower bound \(1 = 2/d\) obtained from the Harris criterion, for all \(q \geq 2\).

To conclude, we have highlighted some interesting properties associated with the inclusion of non-magnetic impurities in three-dimensional frustrated magnets. In particular, a new universality class was shown to appear, with associated critical exponents differing strongly from the effective exponents measured in the pure case. We also gave some indications for a very appealing behavior of the critical exponent \(\nu\), and a large value of \(\eta\). A verification of these effects by independent approaches, in particular perturbative expansions and Monte-Carlo simulations, would be very valuable. At the light of the results presented here, it would be particularly interesting to reconsider the experimental studies on diluted frustrated magnets.

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FIG. 1: Critical exponents of the diluted STA, as a function of the number of spin components. The dotted line corresponds to the lower bound given by Harris criterion.

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[19] Here, small enough means \(d \leq 4\) for systems with continuous order parameters (such as XY or Heisenberg spin systems), and \(d \leq 2\) for discontinuous order parameters (such as Ising and Potts models).
[20] For \(n = 1\) (Ising model), \(G_1(\tilde{x}) = -\ln(cosh(\tilde{x}))\).
[21] We thank P. Lecheminant for comparison with his unpublished results.