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CONTINUOUS PHASE TRANSITION INDUCED BY IMPURITIES IN FRUSTRATED MAGNETS[1]

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We report on recent works aiming at describing the influence of non-magnetic impurities on the phase transitions in frustrated magnets. A two-loop calculation and a renormalization-group approach in the framework of the effective average action show that the phase transition, which is expected to be weakly of first order in the pure case, is turned into a continuous one in presence of impurities.

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1 Introduction

The influence of disorder in solid state physics is a very important, and still debated problem. The first obvious reason is that no experimental sample can be completely free of impurities, defects in the lattice structure, etc. Therefore, if it is natural to consider as a first approximation that the material considered is pure, it is very important to test how the results obtained within this approximation can be altered by the presence of disorder. Second, and more interesting for us, it is now well established that the presence of impurities can induce completely new physical behaviors in the systems. Let us discuss here two examples in the framework of phase transitions, which we are dealing with here.

In some systems undergoing a second order phase transition, taking into account the role of impurities changes the universality class describing this transition. One can then measure two sets of critical exponents, depending on whether there are impurities or not in the system. The paradigm of this phenomenon is the $d = 3$ Ising model, where two sets of critical exponents have been measured experimentally, and computed analytically (see [1] for a review). One is observed in the pure system, and the other when the system is diluted with non-magnetic impurities. There is a slight difference between these two sets of critical exponents. For example, the critical exponent ν, governing the singularity of the correlation length at the critical temperature changes from $\nu_{\rm p} = 0.630$ in the pure system to $\nu_{\rm d} = 0.678$ in the disordered case. This change of universality class can actually be expected from the very general Harris criterion [2, 3], which states that for a very large class of systems with impurities, the critical exponent ν must satisfy

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the bound $\nu_{\rm d} \geq 2/d$. From this, one can infer that in all three-dimensional systems with $\nu_{\rm p} \leq 2/3$ (which is in particular the case for the Ising model), impurities have a drastic role since they must change the critical exponent ν, and therefore change the universality class of the system.

In systems undergoing first order phase transitions, the influence of disorder can even be more dramatic. Typically, one expects the discontinuities which characterize a first order phase transition (*i.e.* the latent heat, the jump of the magnetization) to be reduced when impurities are added [4]. This phenomenon is referred to as the rounding effect of disorder. In some situations, these discontinuities even disappear, and we can then observe the very interesting situation of a continuous phase transition induced by impurities. This phenomenon has been observed in the $d = 2$ q-states Potts model. The phase transition, which is known to be of first order for $q \geq 5$ is turned into a continuous one when some disorder is included in the system (see [5] and references therein). Again, this change of behavior is to be expected for a wide class of systems. Indeed, there is a very general theorem by Aizenman and Wehr [6] which states that for systems with discrete order parameter (such as Ising or Potts models) with some disorder included—for instance a random distribution of the nearest neighbors interaction—the latent heat vanishes. When the degrees of freedom are continuous, such as in XY and Heisenberg spin systems, this theorem holds for any dimension lower than four. Notice that, in principle, there could exist phase transitions with vanishing latent heat but with a jump in the magnetization, which would then be considered as being of first order. However, simple arguments *a la* Landau show that this is unlikely, and the theorem of Aizenman and Wehr indicates that most probably, in low enough dimension, a discontinuous phase transition becomes of second order when impurities are added.

We want to stress the fact that adding impurities, even a small density Δ, changes qualitatively the behavior of the system. This is very surprising, and seems to indicate that, as no sample can be completely free of impurities, the first order behavior of the pure system should never be observed experimentally. This is actually not the case, and one instead expects a crossover from the behavior of the pure system to that of the disordered one. Only in a small range of temperature around the critical temperature—of typical extension $\Delta^{1/\nu d}$—do the impurities influence the physical behavior. This domain of temperature can very well escape to experimental observations for very clean materials.

The phenomenon of second order phase transition induced by impurities have been mainly studied in $d = 2$, where one can use very powerful analytical methods (see [7] and references therein), but not much was done in three dimensions. Moreover, most of the models considered didn't have a direct experimental realization for which such behaviors could be studied. We recently proposed [8] that this phenomenon could be observed in some frustrated magnets, such as stacked triangular antiferromagnets ($CsMnBr_3$, $CsNiCl_3$, etc) and rare earth helimagnets (Ho, Tb). These materials have been very much studied in the past twenty years, and it might well be that the rounding effect of disorder can be observed in such systems.

2 Pure frustrated magnets

Frustration by itself is a very interesting phenomenon in condensed matter physics. It appears when the microscopic degrees of freedom are submitted to competing interactions. Among the simplest realizations of frustration, one finds the stacked triangular antiferromagnets. These materials can be modeled by spins $\vec{S}_i$ on stacked triangular lattices, with two or three-components

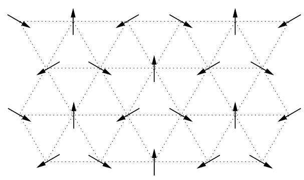

Fig. 1. Ground state of the stacked triangular antiferromagnets.

spins (depending on the anisotropies of the crystal), submitted to antiferromagnetic interaction between nearest-neighbors in the plane. We consider here a direct generalization where the spins have an arbitrary number n of components. The Hamiltonian then reads:

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j, \tag{1}$$

where $J > 0$ describes the strength of the exchange interaction. When building the ground state of the theory, it is easily observed that one cannot minimize simultaneously the energy of interaction of each pair of spin, and the ground state acquires a non-trivial geometrical structure (see Fig. 1). Consequently, the rotational symmetry is completely broken in the ground state, and it was soon understood that a new symmetry-breaking scheme is realized—for an arbitrary number n of spin components, the symmetry-breaking scheme reads $O(n) \times O(2) \to O(n-2) \times O(2)$—and therefore a new universality class was associated with the phase transition undergone by these materials [9, 10]. Moreover, when we look for the soft modes—which govern the long-distance physics—and write down the continuum limit of this theory, we observe that the order parameter is not a simple vector, as in the ferromagnetic-paramagnetic phase transition, but is instead composed of two vectors, noted $\vec{\varphi}_1$ and $\vec{\varphi}_2$. The "φ^4" action then reads:

$$\mathcal{S}(\phi) = \int d^d x \Big[\frac{Z}{2} \mathrm{Tr} \left(\partial\, {}^t\phi . \partial \phi \right) + r\, \frac{\rho}{2} + \frac{u_1}{8} \rho^2 + \frac{u_2}{4} \tau \Big] \tag{2}$$

where we merged the two vectors into a matrix $\phi = (\vec{\varphi}_1, \vec{\varphi}_2)$, and introduced $\rho = \mathrm{Tr}\,({}^t\phi \cdot \phi)$ and $\tau = \mathrm{Tr}\,({}^t\phi \cdot \phi \cdot {}^t\phi \cdot \phi)$. u_1 and u_2 are standard "φ^4" coupling constants, r describes the strength of the mass-like interaction and Z is the field renormalization.

The previous model has been studied in the framework of renormalization group, and some recent works lead to the conclusion that the phase transition should be weakly of first order [11, 12]. This means that the system has a finite correlation length at the phase transition, but so large that some features of continuous phase transitions—*i.e.* universality, power-law behaviors, etc.—should hold approximately. This behavior is in good agreement with the experimental observations and Monte-Carlo simulations, where power-laws are observed, but with a strong dependence of the associated critical exponents on the microscopic details of the system (see [13] and references therein). Associated with this very large correlation length, one also expects a tiny jump of the magnetization, a tiny latent heat that cannot be observed in most experiments and numerical simulations. The order of the phase transition in these systems is however still debated since a six-loop calculation leads to the conclusion that the phase transition is continuous [14].

3 Frustrated magnets diluted with non-magnetic impurities

We now come to the case where some frozen non-magnetic impurities are randomly introduced in the system. At the microscopic level, one can then consider the following Hamiltonian [15]:

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \epsilon_i \epsilon_j \, \vec{S}_i \cdot \vec{S}_j, \tag{3}$$

where ϵ_i equals 0 if a non-magnetic impurity is present at the lattice site i, and 1 otherwise. In order to describe a diluted system, we choose the ϵ_i to be non-fluctuating, uncorrelated random variables. The continuous limit can then be taken, as in the pure case, and one recovers an action similar to Eq.(2), except that the coupling constants $\{Z, r, u_1, u_2\}$ now depend on the variables ϵ_i, and are no more constant in space. One can however average over the disorder, and retrieve a translational-invariant theory by using the replica trick. We refer to the communication of J.K. Wiese in this issue for a more detailed discussion of this method. In our problem, the averaging makes necessary the introduction of a new label l for the fields, which formally runs from 1 to o, and to take the limit $o \to 0$ at the end of the calculation. The "ϕ^4" action then reads [8]:

$$\mathcal{S}(\phi_k) = \int d^d x \left\{ \sum_{l=1}^{o} \left[\frac{Z}{2} \mathrm{Tr} \left(\partial \, {}^t\phi_l . \partial \phi_l \right) + r \, \frac{\rho_l}{2} + \frac{u_1}{8} \rho_l^2 + \frac{u_2}{4} \tau_l \right] + \frac{u_3}{8} \left[\sum_{l=1}^{o} \rho_l \right]^2 \right\}. \tag{4}$$

The four first terms are similar to the ones appearing in the Hamiltonian (2) of the pure system. On the other hand, the last term is new, and describes the influence of disorder on the critical properties of the system. Notice that only this last term couples the different replicas of the field, so that if we set $u_3 = 0$, we recover a theory with o independent replicas of the field, whose interaction is described by the pure Hamiltonian (2).

We now discuss two renormalization group approaches of the theory described by the previous action. The first one relies on a double expansion in powers of the coupling constants and in $\varepsilon = 4 - d$. It enables us to observe the appearance of a new fixed point of the renormalization group, and therefore to test the scenario of the rounding effect of disorder in a controlled way. However, this approach is not reliable when ε is set to 1. Therefore, to study the behavior of the system in the case of physical interest, *i.e.* $d = 3$, we present a calculation in the framework of the effective average action which enables to determine non-perturbative β-functions. This leads to a more precise picture of the physics in $d = 3$.

3.1 Perturbative results

The β functions for the three coupling constants u_1, u_2 and u_3 were obtained by using dimensional regularization and minimal substraction scheme [16]. One can then study the existence of fixed points of the renormalization group, for any number of spin components, and for dimensions close to $d = 4$. Our results are summarized in figure (2). The plane is divided by two curves, which can be calculated within the ε expansion. Above $n_{\mathrm{p}}(\varepsilon) \approx 21.8 - 23.4\varepsilon + 7.09\varepsilon^2$ [17], the pure system exhibits a second order phase transition, governed by a fixed point in the plane $u_3 = 0$. For $n_{\mathrm{p}} \geq n \geq n_{\mathrm{d}}$ with $n_{\mathrm{d}} = 21.8 - 23.4\varepsilon - 37.3\varepsilon^2$, there is no more fixed point in the plane $u_3 = 0$. However there is now a stable fixed point for $u_3 \neq 0$, and the transition becomes of second order because of the presence of impurities. If we naively extrapolate these

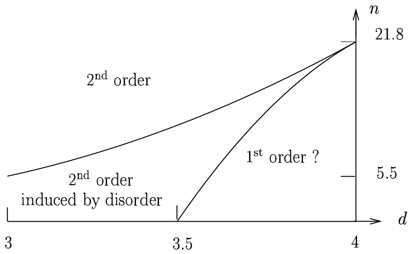

Fig. 2. Order of the phase transition in the (n, d) plane. The extrapolation to $d = 3$, and in particular $n_{\rm d}(d = 3) = 5.5$, is given for indication.

results to $d = 3$, we observe that, in the cases of physical interest *i.e.* for $n = 2$ or $n = 3$, the scenario of second order phase transition induced by disorder is favored. Finally, for $n < n_{\rm d}$, there is no fixed point of the renormalization group, and the transition is expected to be of first order. This last result is very surprising, being hardly compatible with the theorem of Aizenman and Wehr, which states that, in this region, the phase transition should be continuous (see the introduction). It is not yet known how this discrepancy can be resolved, but three possibilities can be proposed. First, it could be that the phase transition is indeed of first order, as predicted by the perturbation theory, but with a vanishing latent heat. This behavior is not very likely, but cannot be discarded so far. Second, the symmetry between the different replicas, which was implicitly assumed to hold could be spontaneously broken. In this case, the action (4) would not give anymore a satisfactory description of the system. It would then be necessary to consider a more general action and to rederive β functions for this system, which may lead to a new stable fixed point. Finally, there could exist a non-perturbative fixed point, unreachable within perturbative expansions. These three possibilities are of great interest, and deserve further analysis.

We want to stress the fact that a two-loop calculation usually enables one to compute a critical value of n up to linear order in ε. However, we observed a particular behavior of the β function in this model, which enables, when taking into account some three loop results for the pure case, to extract the ε^2 coefficient of $n_{\rm d}$ within the two-loop calculation [16].

3.2 In the framework of the effective average action

The results obtained within perturbation theory confirm our expectations concerning the second order transition induced by fluctuations in frustrated magnets. However, this perturbative approach is not fully reliable when extrapolated to $d = 3$, and it is therefore interesting to consider an alternative approach, not restricted to the vincinity of $d = 4$. To this end, we made a calculation in the framework of the effective average action. This method has been successfully applied in many systems, and in particular for physical situations very close to what is considered here (see [13] for a study of the pure frustrated magnets, and [18] for a study of the disordered Ising model, see above). We shall not give a detailed description of this method here, and refer to the communication of Y. Kubyshin in this issue, and to [19] for a review. We used a truncation of the form (4), except that we took into account the "φ^6" terms in order to get more accurate results.

Our main result is that a fixed point of the non-perturbative flow equations is found. By diagonalizing the flow around this fixed point, we are able to determine the critical exponents describing the phase transition governed by this fixed point. In practice, we compute ν and the anomalous dimension η from which the other critical exponents can be deduced thanks to the scaling relations. For $n = 2$, we find $\nu = 0.60$, $\eta = 0.13$, and for $n = 3$, $\nu = 0.64$, $\eta = 0.078$. These numerical result are not fully satisfying when compared with the bound imposed by the Harris criterion. Indeed, for a three-dimensional system, the critical exponent ν should be greater than $2/3$, which is not the case here. However, one can estimate the error within the kind of truncation considered here to be of the order of η [19], and the Harris criterion's bound can be fulfilled within these errors. We expect this discrepancy to be resolved when richer truncations are considered.

4 Conclusion

We studied the influence of non-magnetic impurities on the critical behavior of frustrated magnets. Two complementary approaches lead to the conclusion that the phase transition is of second order in $d = 3$, in the cases of physical interest, because of the presence of the impurities. Some important features remain to study. It would be particularly important to determine with higher accuracy the value of the critical exponents in $d = 3$. To this end, different techniques could be used, going from high loop calculations to Monte-Carlo simulations. A precise determination of the critical exponents could trigger experimental studies of these materials. Concerning the results obtained around $d = 4$, the behavior in the small n region is still not satisfactory, and deserve further work.

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