Continuous Versus First Order Transitions in Compressible Diluted Magnets

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Abstract

The interplay between disorder and compressibility in Ising magnets is studied. Contrary to pure systems in which a weak compressibility drives the transition first order, we find from a renormalization group analysis that it has no effect on disordered systems which keep undergoing continuous transition with rigid random-bond Ising model critical exponents. The mean field calculation exhibits a dilution-dependent tricritical point beyond which, at stronger compressibility the transition is first order. The different behavior of XY and Heisenberg magnets is discussed.

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1 Introduction

The effects of the magneto-elastic coupling (MEC), between the spin and the lattice vibrational degrees of freedom, have been investigated extensively [1-10]. Basic thermodynamics implies that for magnetic systems with a diverging specific heat the presence of the MEC will cause an instability. Therefore the divergence is averted by a preemptive first-order transition. Mean-field theory (MFT) and solutions of simplified models [3-6] have vindicated this conclusion. In particular MFT predicts the existence of a tricritical point separating second- and first- order transitions, as the intensity of the MEC is increased [5]. Other types of behavior were predicted upon changing boundary and other conditions. However, they will not be discussed here [11]. An even better understanding was achieved with the application of the renormalization group (RG) approach to these systems [7-9]. Calculations in $d=4-\epsilon$ dimensions, have shown the behavior to depend crucially on the number of components $m$ of the order-parameter. For example the ferromagnetic continuous transition of rigid Ising-like systems ($m=1$) is fluctuation-driven to a first-order transition once the MEC is accounted for. On the other hand $XY$ ($m=2$) and Heisenberg ($m=3$) systems are unaffected by the compressibility and the MEC is irrelevant [7-9]. This particular aspect is in accordance with the early results since the crossover exponent for the MEC is $\alpha$, the rigid system specific heat exponent and the interaction is relevant for rigid systems with a divergent specific heat, i.e. $\alpha > 0$. 

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Experimentally, the coupling is exhibited by the sensitivity of the critical temperature to an applied external pressure. First-order and continuous transitions, in some cases separated by a tricritical point, were reported in different systems [12-16].

In the present article we shed a new light on the behavior of compressible magnets. We emphasize the drastic role played by quenched bond disorder, such as dilution (obtained by replacing some of the ions by non-magnetic ones). We find that for Ising-like systems the quenched disorder has a crucial effect in preventing the runaway to the first-order transition caused by the MEC in pure systems. This drastic effect of the disorder originates from the so-called Harris criterion: Weak disorder is relevant for rigid systems with positive $\alpha$ (namely precisely the same systems that are affected by the MEC). These disordered rigid systems exhibit a new critical behavior associated with a random fixed-point for which $\alpha < 0$. Hence one possibility is that a weak MEC will not affect their behavior (another possibility being that the MEC has the dominating effect: It drives the transition discontinuous which is then somewhat weakened by the disorder). In the next Section (2) the former heuristic conclusion is confirmed by a detailed RG analysis. In Sec. 3 the MFT is applied and its results are compared with those obtained by the same method for pure compressible magnets. In the last Section (4) the important conclusions are summarized and discussed within the context of other bond-disorder effects in low-dimensional magnetic models.
2 Renormalization group analysis

The momentum-shell RG analysis begins from a continuous-spin Landau-Ginzburg-Wilson Hamiltonian. With $\tilde{\phi}(\vec{x})$ representing the $m$-component spin field and $\vec{u}(\vec{x})$ the d-dimensional local displacement the Hamiltonian is [4,7]:

$$-\beta H = \int d^d x \left\{ \frac{1}{2} r(\vec{x})(\tilde{\phi}(\vec{x}))^2 + \frac{1}{2} \sum_{\alpha=1}^m (\tilde{\nabla} \phi_\alpha(\vec{x}))^2 + u_0(\tilde{\phi}(\vec{x}))^4 + \frac{1}{2} K - \frac{1}{d} \mu (\nabla \cdot \vec{u}(\vec{x}))^2 + \mu \sum_{\nu=1}^d (\tilde{\nabla} u_\nu(\vec{x}))^2 + g(\nabla \cdot \vec{u})(\tilde{\phi}(\vec{x}))^2 \right\}. \tag{1}$$

The first three terms represent the rigid random-bond Ising model. The dilution is accounted for in $r(\vec{x}) = r + \delta r(\vec{x})$, where $r$ is the average of the local random “temperature” $r(\vec{x})$. The local deviations obey

$$< \delta r(\vec{x}) \delta r(\vec{y}) > = < \delta r^2 > \delta(\vec{x} - \vec{y}),$$

(higher moments are irrelevant and so are the omitted disorder-dependent terms in the elastic part of the Hamiltonian). $K$ and $\mu$ are the bulk and shear moduli and $g$ is the MEC. To average over the disorder we use the “$n$ goes to zero” replica trick. After replicating and averaging the local displacements may be integrated out in $< Z^n >$. The outcome is an effective replicated
Hamiltonian depending only the n m-component vector $\vec{\phi}^\alpha$, $\alpha=1,2,...,n$:

\[
- \beta H_{\text{rep}} = \int d^d x \left\{ \sum_\alpha \left( \frac{1}{2} r(\vec{\phi}^\alpha)^2 + \frac{1}{2} \sum_{a=1}^m (\vec{\nabla} \phi_a^\alpha)^2 + u(\vec{\phi}^\alpha)^4 \right) \right\} + \sum_\alpha \frac{v}{V} \left( \int d^d x (\vec{\phi}^\alpha)^2 \right)^2 - \Delta \int d^d x (\sum_\alpha (\vec{\phi}^\alpha)^2)^2 ,
\]

where:

\[
u = u_0 - \frac{g^2}{4 \left\{ \frac{1}{2} K + \left( \frac{d-1}{d} \right) \mu \right\}} ,
\]

\[
v = \frac{1}{4} g^2 - \frac{1}{\left\{ \frac{1}{2} K + \left( \frac{d-1}{d} \right) \mu \right\}} + \frac{2}{K} ,
\]

and

\[
\Delta = 8 < \delta r^2 > .
\]

The initial (and physically acceptable) values obey $u > 0$, $\Delta > 0$, $v < 0$. $V$ is the volume of the system.

The Hamiltonian has three quartic couplings. The flow within the three dimensional subspace of parameters which contains $u$, $\Delta$, and $v$ determines the fixed-point structure of the system. Integrating out small scales
fluctuations, we obtain the recursion relations to order one loop:

\[ \frac{\partial u}{\partial l} = \epsilon u - \frac{m + 8}{6} u^2 + 2\Delta u, \quad (3) \]

\[ \frac{\partial \Delta}{\partial l} = \epsilon \Delta + \frac{mn + 8}{6} \Delta^2 - \frac{m + 2}{3} \Delta u, \quad (4) \]

\[ \frac{\partial v}{\partial l} = \epsilon v - \frac{m}{2} v^2 - \frac{m + 2}{3} uv + \frac{n + 2}{3} \Delta v, \quad (5) \]

One observation is called for at once: the coupling \( v \) cannot feed into the renormalization of the two others because of its special non-local form. Consequently we separate the search for the fixed points (f.p.) into two steps: We look first for the f.p. in the \( u-\Delta \) directions. Secondly, with these f.p. values for \( u \) and \( \Delta \) inserted into Eq. (5) we look for its fixed-points. The first step is analogous to the analysis done in the study of rigid random-bond models. The results are also \( m \)-dependent [17]. For the Ising model the pure f.p. is unstable towards the inclusion of the disorder coupling \( \Delta \), while it is stable for systems with \( m > 1 \) [17,18]. We therefore discuss the results for these cases separately.
2.1 Ising model (m=1)

The stable f.p. in the u-Δ plane is the so-called Khmel’nitskii’s f.p. [18] at which both u and Δ are of order \( \sqrt{\epsilon} \). We therefore have to check the stability of this f.p. while switching on \( v \). To that goal we insert the values of the f.p. \( u^* = \sqrt{\frac{6}{53}} \epsilon^\frac{1}{2} \) and \( \Delta^* = \frac{3}{4} u^* \) to Eq. (5). These values were obtained from two-loop calculations [18,19]. For \( v \) close to zero the term in \( v^2 \) is negligible and thus we have:

\[
\frac{\partial v}{\partial l} = (\epsilon - u^* + \frac{2}{3} \Delta^*)v = -2 \sqrt{\frac{6}{53}} \epsilon^\frac{1}{2} v.
\] (6)

Terms of order \( \epsilon \) were neglected compared with \( \sqrt{\epsilon} \). It should be noticed that the crossover exponent for \( v \) is \( \alpha \) of the rigid random-bond system. This is contrary to the case in which a random-field is applied to the random-bond system and for which the crossover exponent is not \( \gamma \) of the bond-disordered model [20]. Indeed, in the present case the \( v \) term is the square of the internal energy (per unit volume) and hence has \( \alpha \) as its scaling exponent. Our finding \( dv/dl < 0 \) implies that this fixed point is the stable one and hence is describing the critical behavior of this system (at least within the renormalized perturbation theory which starts from weak couplings). We thus conclude that elastic random-bond Ising systems will exhibit, at their critical point, the critical exponents of the rigid random-bond Ising system. If the MEC coupling \( v \) is large and that of the disorder \( \Delta \) is small, the initial
flow will be towards larger $v$. The stability boundary may be reached before the flow reverses itself to smaller values. In this case a first-order transition is still possible and the continuous transition will be attained (through a tricritical point) at a finite strength of the disorder. That is very different from the behavior in absence of disorder for which it was found that the elasticity is relevant at the order $\epsilon$ Wilson-Fisher f.p. (of the pure-rigid model [7,8]) and drives the transition first-order. The flow diagram is schematically depicted in Fig. 1.

2.2 Continuous spin models ($m > 1$): XY, Heisenberg, etc.

For these models with continuous symmetry of the order parameter the stable f.p. in the $u$-$\Delta$ plane is that of the pure system. We therefore have to insert the values at this f.p. $u^* = \frac{6\epsilon}{m+8}$ [17] into Eq. (5):

$$\frac{\partial v}{\partial l} = (\epsilon - \frac{6(m+2)}{3(m+8)}\epsilon)v = (\frac{4-m}{m+8})\epsilon v, \quad (7)$$

Although $dv/dl$ is positive for $m < 4$ and small $\epsilon$ at the $v = 0$ f.p., it is again given by $\alpha$ of the rigid (and pure for the considered) systems. As discussed above this is a general relation which holds to all orders in $\epsilon$. It is known [17] that $\alpha$ becomes negative for larger values of $\epsilon$ and is definitively so at $\epsilon = 1$ for all $m > 1$. Therefore $dv/dl$ is negative in 3d and the same f.p. of the
pure and rigid systems also describe their critical properties in presence of
both disorder and compressibility (and their exponents remain unchanged).

3 Mean Field Theory

To go beyond the renormalized perturbation expansion we need to have re- 
course to mean-field theory (MFT), although its results are always to some 
extent questionable (e.g. they are insensitive to the dimensionality of the 
embedding space). However, we may gain some insight by comparing within 
the same approach the predictions for the critical behavior with and without 
dilution.

MFT is applied to the lattice model with $\vec{S}^2 = 1$ on every site. We 
choose a somewhat simplified (Domb’s) model which was shown [3, 5] to 
capture the essential physics. In this model all nearest-neighbor exchange 
interactions are strengthened (or weakened) by the same amount depending 
on the average inter-site distance. The deviation in this distance is pro-
portional to the change in the volume fraction $w = V/N$ ($N$ is the number of 
sites) from its average $w_0$.

The Hamiltonian contains two contributions: the elastic and the mag-
netic. The elastic part is:

$$H_{el} = \frac{N\phi}{2}(w-w_0)^2,$$  (8)
where $\phi$ is proportional to the elastic constant. The magnetic part is [3]:

$$H_{mag} = \sum_{i,j} J_{i,j}(w) S_i S_j,$$

where we have chosen $S_i$ to be a scalar (Ising spin) keeping in mind that MFT yields similar results for m-vector spins. The nearest-neighbor couplings are given by:

$$J_{i,j}(w) = \epsilon_{i,j} \{ J_0 + J_1 (w - w_0) \},$$

$\epsilon_{i,j}$ are independent random variables with the distribution $p(\epsilon) = x \delta(\epsilon) + (1 - x) \delta(\epsilon - 1)$, where $x$ is the concentration of non-diluted bonds (similar results will be obtained for either site or bond dilution). $J_1$ is the coefficient of the part which depends on the inter-site distance (only the dominant, linear, dependence has been kept).

It is straightforward to integrate out the volume fluctuations. The remaining effective Hamiltonian depends only on the spin degrees of freedom:

$$-\beta H_{eff} = \beta J_0 \sum_{i,j} \epsilon_{i,j} S_i S_j + \frac{\beta J_1^2}{2N\phi} \left( \sum_{i,j} \epsilon_{i,j} S_i S_j \right)^2.$$

Introducing mean-fields, both terms are reduced to single-spins ones. Expanding the free energy and performing the average over the disorder yields
the following effective mean-field Hamiltonian:

\[-\beta H_{MF} = \beta J_0 x cm \sum_i S_i - \frac{N}{2} \beta J_0 x cm^2 + \beta \frac{J_1^2}{4\phi} x^2 c^2 m^3 \sum_i S_i - \frac{N}{8\phi} \beta J_1^2 x^2 c^2 m^4,\]

(12)

where c is the coordination number of the lattice and here m is the magnetization per site. From this Hamiltonian all thermodynamic properties can be calculated. In particular for the averaged free-energy we obtain:

\[-\beta \overline{f}_{MF} = \lim_{N \to \infty} \frac{1}{N} \ln Z = -\frac{\beta J_0 x cm^2}{2} - \frac{\beta J_1^2 x^2 c^2 m^4}{8\phi} + \ln \cosh\left\{\beta J_0 x cm + \frac{\beta J_1^2 x^2 c^2 m^4}{4\phi}\right\}.\]

(13)

The critical temperature is given by that at which the \( m^2 \) coefficient vanishes: \( kT_c = xcJ_0 \). The transition becomes discontinuous when the \( m^4 \) coefficient becomes negative. Therefore the tricritical point is at \( kT_c = xcJ_0 \) and \( J_1^2 = \frac{2J_0^2 \phi}{3kT_c} \). We see first that within MFT the critical temperature depends only on the dilution with the same dependence as that of the rigid system. The value of \( J_1/J_0 \) beyond which the transition turns first-order does depend on the dilution: The more diluted is the system the larger this parameter must be in order to change the order of the transition. Hence the regime of second-order is enlarged at the expense of the first-order one the more diluted the system is. The phase diagram is drawn in Fig. 2. This trend is consistent with the RG results for the Ising systems in which a first-order transition was turned
second order by the dilution.

4 Conclusions

To summarize, we have shown that disorder (e.g. dilution) has a crucial role in compressible Ising magnets: While pure systems are driven first-order by coupling spin fluctuations to the elastic degrees of freedom, none of that happens in disordered systems. Their critical properties are insensitive to the compressibility and continue to exhibit a random-bond continuous transition. This behavior is consistent with that of the specific-heat. Indeed, the Harris’s [21] and other [17,22] arguments imply that $\alpha$ of the pure system is also the crossover exponent for the dilution, which is therefore relevant for Ising systems (and irrelevant for $m > 1$ vector-models).

Consequently, Chayes et al. [23] have shown that in any random system $\alpha$ is negative. Hence we reach the general conclusion that the compressibility cannot be relevant at a second-order transition of a random system. Our conclusions are also consistent with those of Refs. [24]. There it was shown that bond-disorder suppresses (in $d = 3$) any tricritical point (it eliminates it in $d = 2$ and therefore 2d compressible magnets undergo always a continuous transition in the presence of disorder).

Although the crossover from one universality class to another is slow ($\alpha$ being a small exponent), compressibility and bond-disorder are present in many physical systems. Therefore it will be very worthwhile to observe
experimentally the effects of dilution in particular on the transition in compressible magnets with uniaxial anisotropy.

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FIGURES CAPTIONS

Fig. 1. The three-dimensional flow diagram with the fixed points:
(A) Pure-Rigid and (B) Disordered-Rigid.

Fig. 2. Schematic mean-field phase diagram ($Y \equiv \frac{j^2}{\varphi}$).