Ordered Phase and Field-Induced Domains in a Short-Range Ising Spin Glass

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Abstract

Using a microscopic numerical approach suitable to describe disordered antiferromagnets, with application to \( \text{Fe}_x \text{Zn}_{1-x} \text{Fe}_2 \), it is shown that the characteristics of the spin glass phase found for \( x = 0.25 \) is much in agreement with the scenario predicted by the scaling theory of the droplet model.

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The Edwards-Anderson (EA) model[1] has become the prototype model used to perform most theoretical studies of spin glasses (SGs). The central feature here is to capture the two essential ingredients, namely disorder and frustration. The latter is introduced by competing ferromagnetic (F) and antiferromagnetic (AF) interactions, while the former requirement is built into the model by allowing the exchange couplings to have a given probability distribution. A simple solution[2] of the model was attempted by assuming infinite-range exchange interactions (SK model), but it was later shown[3, 4] to be a quite hard and complex task. This rather unusual mean-field theory is characterized by ultrametric-based hierarchy, with infinite degenerate ground states unrelated by any obvious (if any) symmetry. This picture proved to be of undoubted importance in several fields such as biology and optimization problems[5], where large effective coordination numbers mimic a high-dimensional space. The question we address, however, is that related to the original motivation: is the mean-field theory a good starting point for real short-range (Ising for simplicity) three-dimensional SGs? This question gave rise to several controversies as a more phenomenological approach, namely the “droplet model”[6, 7], offered a quite distinct alternative scenario. The droplet model is based on numerical results of the short-range EA model, supplemented by scaling and renormalization-group ideas. In particular, it predicts a nondegenerate ground state, except for the trivial up and down possibilities. Moreover, in the droplet picture the SG phase is destroyed by an applied external magnetic field ($H$) and thus, contrary to the mean-field prediction, no equilibrium de Almeida-Thouless (AT) line exists. Experimental[8] and theoretical studies[9] facing these controversies have found it difficult to announce clear-cut results, in part because of the very slow dynamics plaguing these systems, a characteristic shared by both competitive descriptions.

In this work we study the above-mentioned problems using a direct microscopic approach suitable to describe short-range three-dimensional insulating Ising SGs. A random-site dilution is thus used instead of the random-bond approach of the EA model. In fact, we shall parametrize our model Hamiltonian in the expectation that
a description of the experimental observations[10] on the compound $Fe_xZn_{1-x}F_2$, as a function of dilution $x$, is achieved.

Very recently, we showed[11] that the presence of a very small frustrated interaction is the mechanism underlying the appearence of the SG phase at $H = 0$ in $Fe_{0.25}Zn_{0.75}F_2$. Here we extend our study and calculate the spin-spin correlation function in the ordered SG phase and the characteristics of the field-induced domains both in the SG and in the “random field Ising model” (RFIM) phases. While the RFIM phase is very stable under an applied field, its effect on the SG phase is dramatic regardless of the value of the field. Our results are in agreement with the scenario predicted by the droplet model, including the chaotic behavior of the correlation function as the spin distance varies at constant $T$. The main quantitative result is the value of the exponent governing the $H = 0$ SG ordered phase, $y_T = 0.19 \pm 0.03$. Moreover, we show that an irreversibility (AT) line exists regardless of the presence of frustration. We conclude that these lines are metastable lines, as also supported by the droplet model, and that the SG phase is indeed destroyed by an applied field, as recently experimentally reported for the compound $Fe_{0.5}Mn_{0.5}TiO_3$ [12].

**Formal procedure:** we perform numerical simulations of the iterative set of equations of the local (site-by-site) mean fields (LMFs) derived from the microscopic Hamiltonian

$$
\mathcal{H} = \sum_{<i,\delta \ell>} J_\ell \mathcal{E}_i \mathcal{E}_{i+\delta \ell} S_i S_{i+\delta \ell} - \mu_o \sum_i \mathcal{E}_i S_i H,
$$

where $S_i = \pm 2$ (as in $Fe^{+2}$), $\mathcal{E}_i = 0, 1$ and $\ell$ is summed over the three nearest-neighbor exchange interactions $J_\ell$ of the centred tetragonal lattice of $Fe_xZn_{1-x}F_2$ [10]. We choose the values of the exchange constants by keeping unaltered the experimental ratios $j_1 = J_1/J_2 = -0.013, j_3 = J_3/J_2 = +0.053$ and such as to fix the Néel temperature of the pure system, $T_N(x = 1) = 77.8K$. This LMF technique has proven[13] very efficient in describing inhomogeneous and disordered systems. The thermally averaged local spin $m_i$, results from the free energy minimization in
the form ($\mathcal{E}_i = 1$):

$$m_i = \langle S_i \rangle_T = 2 \tanh\{2h_i/KT\},$$

(2)

where the local field at site $i$ is given by

$$h_i = -\frac{1}{2} \sum_{\delta_t} J_{i+\delta_t} \mathcal{E}_{i+\delta_t} m_{i+\delta_t} + \mu_0 H.$$  

(3)

Introducing $C_{ij}(T) = \langle S_i S_j \rangle_T - m_i m_j$, we find the LMF expression

$$\langle S_i S_j \rangle = 4 \frac{\cosh[2(h_i + h_j)/KT] - \cosh[2(h_i - h_j)/KT]}{\cosh[2(h_i + h_j)/KT] + \cosh[2(h_i - h_j)/KT]}.$$  

(4)

The spin-spin correlation function of interest is then $G_T(r_{ij}) = \langle C_{ij}^2 \rangle_{av}$, where $av$ indicates an average over distinct random spin configurations, such that $\langle C_{ij} \rangle_{av} = 0$. The staggered magnetization is defined by

$$M_S(T, x) = (2/N) \sum_i \mathcal{E}_i m_i,$$

(5)

with $i$ summed over a given sublattice, and the SG-EA order parameter by

$$Q(T, x) = (1/N) \sum_j \mathcal{E}_j \langle S_j^2 \rangle_T,$$

(6)

with $j$ taken through the whole lattice.

We choose a random initial configuration $\{S_i, \mathcal{E}_i\}$ in the high-$T$ paramagnetic phase and average over 50 independent runs. The system is cooled by an amount $\Delta T$ (we take $\Delta T = 0.05K$ for the (H,T) phase diagram, and $\Delta T = 1K$ otherwise), using (2) and a proper convergence criterion[11, 13], down to $T = 2K$ and heated back using the same amount of $\Delta T$. We take $N = 2 \cdot 30^3$ sites and use periodic boundary conditions.

**Numerical data and analysis:** first we point out that our data correspond to a proper time scale in which a quasi-equilibrium state is achieved at $H = 0$. In Fig.1(a) we illustrate a SG ordered phase configuration through part of a randomly chosen sheet: $x = 0.25$, $T/T_N(x = 1) = 0.18$ and $H = 0$. The local-field distribution corresponding to this state is shown in Fig.1(b). As evidenced from the inset, competitive local fields exist only in the presence of frustration. In fact, the effect of frustration
manifests itself only in the high dilution regime ($x < 0.5$) and causes domains of reversed spins surrounded by domain walls already when the system behaves as a RFIM ($x = 0.48$) [11]. This spin reversal effect completely changes the balance of forces, thus causing the appearence of competitive local fields, particurlarly near the percolation threshold in which case a full SG phase emerges.

In the scaling theory[6, 7] of the droplet model the SG ordered phase is characterized by the exponent associated with the thermal eigenvalue, $(T(L)/J(L)) \sim L^{-y_T}$, of the $T = 0$ fixed point, where $J(L)$ is an effective exchange interaction. It also measures the scale of the free energy, $F = Y(T)L^{y_T}$, associated with the thermally activated droplets of reversed spins surrounded by domain walls. The average size of the domains increases as the temperature decreases, with $Y(T = 0) \sim J$. We have measured the correlation function $G_r$, for $x = 0.25$, and assumed a scaling dependence, $G_r(T) = f(r) \exp(-r/\xi)$, where $\xi \sim T^{(1/y_T)}$, valid in the low-temperature region of the $H = 0$ SG ordered phase. The fitting of the data is shown in Fig.2: we find $y_T = 0.19 \pm 0.03$, in very good agreement with the estimates[6] using $T = 0$ renormalization-group treatments of the short-range EA model. The data are for pairs of spins (ten pairs in this case) inside the same domain. For pairs with spins in different domains the correlation is null. Notice that the $T$-behavior of $G_r(T)$, shown in the inset of Fig.2, confirms a finite-$T$ phase transition. In Fig.3(a) we plot the temperature dependence of $< S_i S_j >_T$, with sites $i$ and $j$ randomly chosen on the lattice. Different behaviors are seen, including a change of sign, indicating spin reversal by thermal activation of domains. On the other hand, the chaotic behavior of $< S_i S_j >_T$ as a function of spin distance at $T/T_N(x = 1) = 0.18$ is nicely displayed in Fig.3(b). The Lyapunov exponent associated with this behavior is predicted[7] to be $\zeta = d_s/2 - y_T$, where $d_s$ is the fractal dimension of the domain walls. $\zeta$ is exactly one in $d = 1$ and expected to change very little with the system dimensionality. Last, we should emphasize that below $T/T_N(x = 1) = 0.18$ there are practically no spin reversal and thus for all practical purposes the spin configuration of Fig. 1(a) is the $H = 0$ SG ground state for a given initial configuration $\{S_i, \mathcal{E}_i\}$ in the
paramagnetic phase; \{-S_i, \mathcal{E}_i\} leads to a ground-state configuration with all spins reversed. Moreover, for a quenched disorder configuration \{\mathcal{E}_i\}, the ground state remains the same regardless of the spin paramagnetic configuration \{S_i\}, i.e., the SG state is self-averaged\[9\].

We now turn to study the system in the presence of an applied field. In a field-cooled (FC) cycle random fields of strong magnitudes induce SG-like states, regardless of the presence of frustration. These spin structures are formed by domains of the two (up and down) equivalent $H = 0$ SG-ground states\[6,7\], i.e., the original configuration of Fig.1(a) breaks up into domains of length scale, $L_H \sim (J/H)^{1/(d/2-y_T)}$, which independently align with the field. It means that the field is a relevant scaling variable governed by the (positive) exponent $y_H = d/2 - y_T$, $(H(L)/J(L)) \sim L^{y_H}$. The spin structures of these SG-like states are illustrated in Fig. 4(a) by indicating the domains of reversed spins ($\ominus$) relative to the $H = 0$ SG ground-state (Fig. 1(a)), for $x = 0.25, T/T_N(x = 1) = 0.18$ and $H = 1.0 G$. The associated distribution of local fields are shown in Fig. 4(b). The inset of Fig. 4(b) shows that, in the absence of frustration, a zero-field-cooled (ZFC) cycle induces a metastable long-range highly nonuniform AF order as a result of the local AF interactions predominating in the system. We should stress that we have access to the microscopic local spin values on our chosen sheets. It is thus observed that the local spin values on the structure of Fig. 4(a) and on the mentioned AF structure (inset of Fig. 4(b)) are the same of those in Fig. 1(a) (for any $H < 10^3 G$), except for a change of sign for those spins suffering a spin reversal and a small magnetization component in the field direction (experimentally called\[10\] $M_{FC}$ and $M_{ZFC}$, respectively). This is so because our fields states were “prepared” using the same initial configuration of Fig. 1(a).

The characteristics of these field-induced states can also be studied by measuring the effect of frustration on the EA-SG order parameter. In Fig.5(a) we see the qualitative change of behavior as a result of an applied field in a FC cycle: while in the $H = 0$ state frustration is a fundamental ingredient ($Q = 0$ if $j_3 = 0$), under a field, regardless of its value, frustration decreases the $Q$ value! Saturation of $Q$
is achieved at about $10^2T$. To further evidence the special character of the $H=0$ SG phase found for $x=0.25$, we have also studied the effect of frustration on the system for $x=0.48$, a regime dominated by random-field effects on top of the long-range AF ordering. In Fig.5(b) we see that frustration always decreases $Q$, even for $H=0$. The effect of frustration peaks at an intermediate temperature, because in this situation neither full ordering nor full disorder predominates in the system. Finally, in Fig.6 we display the field-induced AT - irreversibility lines ($\bullet$) obtained by the loci of the points in which $M_{FC}$ differs from $M_{ZFC}$. We see that exponents compatible with the experimental results are found regardless of the presence of frustration. As we see from the insets of Fig. 6(a) and 6(b) the FC ($\cap$) and ZFC ($\Diamond$) correlation functions, for $H=0.5G$, peak at a temperature below the irreversibility lines, much in agreement with the $H=0$ correlation function in the presence of frustration. The data are for sites in the same domain. In the absence of frustration, however, the $H=0$ correlation function is null (inset of Fig. 6(a)). These results show that in our model for a highly disordered magnetic system, metastable “glassy” states, characterized by the domains of up and down $H=0$ spin configurations of a SG state at a fixed temperature, are induced by an applied field as a result of the strong random fields generated in the system[14]. The effect of frustration is only relevant at very low fields, in which case the approach to SG criticality is only felt by the frustrated system. Though a specific low-temperature SG configuration depends on a given initial paramagnetic configuration \{$S_i, E_i$\}, the ordered phase is univocally characterized by the thermal eigenvalue $y_T$ of the $T=0$ fixed point.

In conclusion, we have presented results based on a local mean-field numerical simulation of disordered AFs, with application to $Fe_xZn_{1-x}F_2$, describing several features of these systems as a function of concentration. In particular, for a concentration near the percolation threshold, the system exhibits a SG phase with a scenario in agreement with the scaling theory of the “droplet” model.

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**Figure Captions**

Fig.1. (a) Part of a SG "ground-state" spin configuration: $x = 0.25$, $T/T_N(x = 1) = 0.18$ and $H = 0$; $\square$ ($\blacksquare$) indicate up (down) spins; $\circ$ indicate zero local spins. (b) Local field distribution of the SG "ground state".

Fig.2. Best fitting of the low $T$-dependence of the correlation function: $G_r(T) = f(r) \exp(-r/\xi)$, $\xi \sim T^{(1/y_T)}$, yielding $y_T = 0.19 \pm 0.03$. The inset shows the peak of $G_r(T)$ at the freezing temperature $T_f$.

Fig.3. (a) $T$-dependence of $<S_iS_j>_T$, with sites $i$ and $j$ randomly chosen on the lattice. (b) Chaotic behavior of $<S_iS_j>_T$ as a function of spin distance at $T/T_N(x = 1) = 0.18$.

Fig.4. (a) Part of a FC spin configuration: $x = 0.25$, $T/T_N(x = 1) = 0.18$ and $H = 1G$; $\square$ indicate spin reversal relative to the SG "ground state" of Fig. 1(a). (b) Local field distribution of a FC spin configuration. The inset shows a ZFC local field distribution in the absence of frustration.

Fig.5. Effect of frustration on the $T$-dependence of the EA order parameter for several values of fields (magnitude in Tesla): (a) FC cycle for $x = 0.25$; (b) ZFC cycle for $x = 0.48$.

Fig.6. Field-induced AT irreversibility lines: dashed lines indicate experimental estimate of the crossover exponent, $\phi \approx 3.4$; dot-dashed lines indicate the AT value, $\phi = 3.0$; full lines are best-fitings. The insets show the $T$-dependence of the correlation function: $\bullet$ indicate data at $H = 0$; $\square$ ($\circ$) are FC (ZFC) data at $H = 0.5T$; (a) in the absence of frustration, $\phi = 3.6 \pm 0.9$ (notice that $G_r(T)$ is null at $H = 0$); (b) in the presence of frustration, $\phi = 3.8 \pm 0.6$. 
\( P(h_i) \)

\( x = 0.25 \),

\( H = 0 \),

\( T/T_N(1) = 0.18 \)
$G_r(T) \cdot (10^5)$ vs. $T/T_N(x=1)$

Inset:

$x = 0.25$
$H = 0$
\[ \frac{S_i S_j}{S_i S_j} \]

\[ x = 0.25 \]

\[ H = 0 \]

\[ j_3 = 0 \]

\[ T/T_N(x=1) \]

(a)

(b)
\( P(h_i) \)

\( x = 0.25 \)

\( H = 1G, FC \)

\( T/T_N(1) = 0.18 \)
$Q_{(j)} - Q(0)$

$x = 0.25$

$F C$

$T/T_N(x=1)$

$x = 0.48$

$Z F C$

$T/T_N(x=1)$

(a)

(b)
$T_{irrev}/T_N(x=1)$

(a)

$T_{irrev}/T_N(x=1)$

(b)