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Field dependence of the transverse spin glass phase transition: Quantitative agreement between Monte Carlo simulations and experiments

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The field dependence of the transverse spin glass phase transition temperature, $T_{xy}(B)$, has been determined both for $a-Fe_xZr_{100-x}$ (x = 90, 91, 92, and 93) using muon spin relaxation and for the bond-frustrated nearest neighbor ±J Heisenberg spin glass using Monte Carlo simulations. In both cases, we find $T_{xy}(B) \propto 1/B$, providing direct, quantitative agreement between experiments and simulations. © *2012 American Institute of Physics*. [doi:10.1063/1.3671432]

Experiments and numerical modeling can yield complementary insights into the magnetic behavior of Heisenberg spin glasses. While numerical models can be used to isolate specific physics within the problem, results must be validated by direct comparison with experimental observations. The zero field magnetic phase diagrams derived from the two approaches are in good agreement and show that a ferromagnet exhibits the initial effects of exchange frustration by developing a second transition below T_C, where spin components perpendicular to the magnetization order as a spin glass at T_{xy}.[1–4] By tuning the chemistry in real materials or by tuning the distribution of interactions in the numerical models, the degree of the frustration may be increased, leading to both a decrease in T_C and an increase in T_{xy} (see Fig. 1). Eventually, the two transitions merge and only a spin glass state remains below the spin glass transition temperature T_{sg}.

The topology of this magnetic phase diagram, where ferromagnetic and transverse spin glass order co-exist, is very similar to that of the Heisenberg spin glass model studied in the mean field approximation by Gabay and Toulouse (GT).[5] Unfortunately, interpretations of experimental data in terms of this mean field phase diagram have, in the past, suffered from the long held view that spin glass phase transitions occur only at zero temperature for realistic, three-dimensional (3D) Heisenberg spin glass models with short range interactions.[6] However, it has recently been demonstrated that a spin glass transition does indeed survive at finite temperatures in 3D for vector spins.[4,7–11] While the *qualitative* similarity between theory and experiment apparent in Fig. 1 is remarkable, there remains no way to *quantitatively* map the two phase diagrams onto one another to assess the direct applicability of the model toward an understanding of the material, due to both the many unknowns in the experimental systems (e.g., distributions of exchange interactions and moments) and the overall simplicity of the numerical model.

We found previously in a—$Fe_{92}Zr_8$ that a simple $1/B$ scaling law captures the field dependence of T_{xy} for $B = 0-7$ T.[12,13] This behavior pointed to an opportunity to establish a clear link between experimental data and the theoretical phase diagram. Our comparison here between $T_{xy}(B)$ for a—Fe_xZr_{100-x} determined using muon spin relaxation (μSR) for $x = 90$, 91, 92, and 93 and $T_{xy}(B)$ from large scale Monte Carlo simulations of the ±J Heisenberg spin glass model exhibits *identical* $1/B$ scaling. This scaling is remarkably robust, holding over a large range of magnetic fields strengths, where T_{xy} decreases by a factor of five and clearly demonstrates a novel, quantitative agreement between experiment and theory.

Experimental determination of $T_{xy}(B)$[12,13] yielded the following approximate scaling form:

$$T_{xy}(B) = T_{xy}(0)\left(1 - \frac{B}{B + A_{xy}}\right), \tag{1}$$

where A_{xy} is a constant. In replica mean field theory,[5] T_{xy} corresponds to the GT line (T_{GT}),

$$T_{GT}(B) = T_{GT}(0)(1 - A_{GT}B^2). \tag{2}$$

Below T_{GT}, mean field theory predicts a second line of transitions, the Almeida-Thouless (AT) line,[5,14] where the replica symmetry of the model is spontaneously broken,

$$T_{AT}(B) = T_{AT}(0)(1 - A_{AT}B^{2/3}). \tag{3}$$

A_{GT} and A_{AT} are scaling constants. The concave down form of Eq. (2) is inconsistent with the experimental form, while the $B^{2/3}$ dependence of Eq. (3) differs from the observed B^{-1} form.[12,13]

The field dependence of T_{xy} was measured by μSR experiments performed at the M20 beamline at TRIUMF. Sample preparation, sample mounting, and other experimental details, including data analysis, are reported elsewhere.[3,12,13,15] A magnetic transition is observed by either the emergence of a static local field (at T_C or T_{sg}) or as an additional contribution to the pre-existing static field due to the magnetization (at T_{xy}).[15] Furthermore, a phase transition (T_C, T_{xy}, or T_{sg}) is also associated with a peak in the muon

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depolarisation rate (λ) caused by critical fluctuations.[3,16] μSR is therefore unique in that it provides unambiguous identification of the transitions through simultaneous measurement of both the static and the dynamic magnetism.

To model a spin glass with coexisting ferromagnetic and spin glass order, we studied the well known ±J Heisenberg spin glass model with the Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} S_i \cdot S_j - B \sum_i S_i \cdot \hat{z}. \tag{4}$$

Classical vector spins $\mathbf{S_i}$ are located on the vertices of a 3D simple cubic lattice of linear dimension L containing $N = L^3$ spins with periodic boundary conditions. Exchange bonds between nearest neighbor spins take the value $J_{ij} = \pm 1$ with probability $P(+) = 1 - x$ and $P(-) = x$, respectively. At $x = 0$, the model reduces to the well understood classical Heisenberg model with $T_c = 1.4429(1)\, J$.[17,18] The phase diagram for the model with $B = 0$ is shown in Fig. 1. Complete details regarding simulation techniques and equilibration conditions are provided in Ref. 4.

The quantities measured in order to determine the model phase diagram are wave vector-dependent susceptibilities $\chi(\mathbf{k})$, from which the correlation lengths[4,7–9,11] are calculated using the definition

$$\xi = \frac{1}{2\sin(|\mathbf{k}_{\min}|/2)} \left(\frac{[\langle \chi(0) \rangle]}{[\langle \chi(\mathbf{k}_{\min}) \rangle]} - 1 \right)^{1/2}, \tag{5}$$

where $\mathbf{k}_{min} = (2\pi/L, 0, 0)$ is the smallest wavevector allowed by the choice of boundary conditions, $\langle\rangle$ represents a thermal average, and [] an average over the disorder. Above a transition ξ is constant, while below it, $\xi \sim L^{d/2}$. At a phase transition, however, $\xi \sim L$, and so plots of ξ/L for different L are expected to cross at the transition temperature.[4,7–11]

For a vector spin glass, $\chi(\mathbf{k})$ is determined by simulating two real replicas of the system α and β and calculating the overlap tensor $q_i^{\mu,\nu} = S_i^{\mu,\alpha} S_i^{\nu,\beta}$, with $\mu, \nu = x, y, z$ the three Cartesian components of $\mathbf{S}_i$. For a transverse spin glass, the definition of the overlap tensor is altered such that only the components of $\mathbf{S}_i$ transverse to the magnetization $\mathbf{m}$ are considered, $S^{\alpha}_{i,\perp} = S^{\alpha}_i - S^{\alpha}_i \cdot \mathrm{m}^{\alpha}/|\mathrm{m}^{\alpha}|$, with $\mathrm{m}^{\alpha} = \mathrm{m}^{\alpha}_x \hat{x} + \mathrm{m}^{\alpha}_y \hat{y} + \mathrm{m}^{\alpha}_z \hat{z}$ and $m^{\mu,\alpha} = N^{-1} \Sigma_i S_i^{\mu,\alpha}$. $\chi(\mathbf{k})$ is then given by

$$\chi(\mathrm{k}) = \mathrm{N}^{-1} \sum_{\mu,\nu} \sum_{\mathbf{i},\mathbf{j}} \mathbf{q}^{\mu,\nu}_{\mathrm{i},\perp} \mathbf{q}^{\mu,\nu}_{\mathrm{j},\perp} \mathbf{e}^{\mathbf{i}\mathbf{k}\cdot\mathbf{r}}, \tag{6}$$

where $\mathbf{r}$ is the vector connecting sites i and j.

ξ has been determined for the transverse spin glass phase at $x = 0.15$ for $L = 4$, 6, 8, 10, and 12 with $B = 0$, 0.01, 0.03, 0.1, 0.3 0.6, and 1.0, each averaged over 500 configurations of disorder. For each (L,T,B) data point, 10^4 over-relaxed Monte Carlo updates (OR-MCSs) were used prior to and during the thermal (time) average that has been shown previously[4] to yield results that are well equilibrated (each update consists of N Metropolis updates and 5 N over-relaxation[19] updates). The ξ curves for all the (L,T,B) data points studied are shown in Fig. 2, and all show clear crossings. T_{xy}

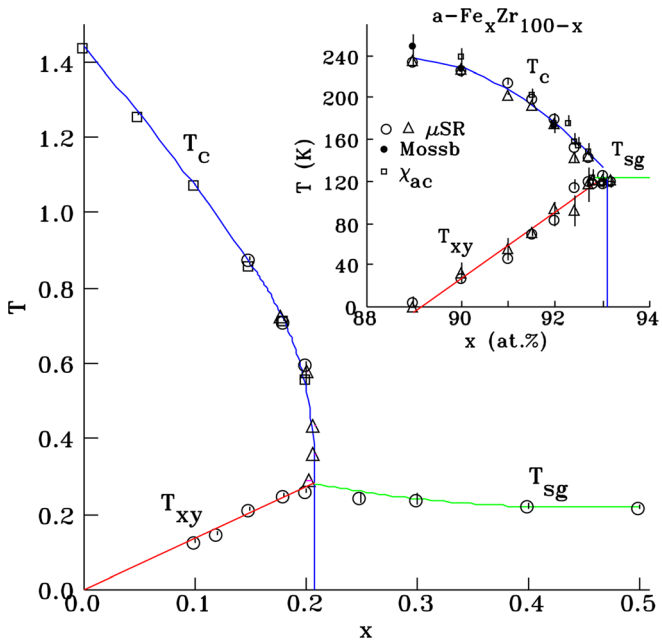

FIG. 1. (Color online) x-T phase diagram of the ±J bond-frustrated Heisenberg model in three dimensions (where x is the fraction of antiferromagnetic bonds, i.e., J = −1). The T_C line separates paramagnetic (PM) and ferromagnetic phases. The line of spin glass transitions T_{sg} separates the PM phase from the spin glass (SG) phase. Below the T_{xy} line, SG order develops transverse to the magnetization. T_C was identified using different numerical criteria (○, Δ, □; for details, see Ref. 4). The same topology is exhibited by the experimental phase diagram of a—Fe_xZr_{100-x}[3] (inset).

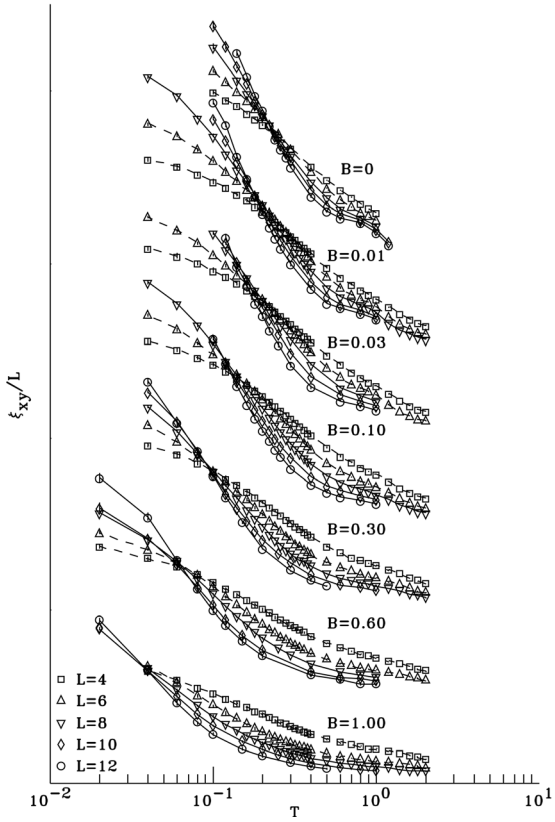

FIG. 2. Crossing of the ξ_{xy}/L data for simulation system sizes of $L = 4$, 6, 8, 10, and 12 at a concentration $x = 0.15$, with magnetic fields $B = 0$, 0.01, 0.03, 0.1, 0.3, 0.6, and 1 (data have been shifted vertically for clarity). Solid lines through $L > 6$ data show clear crossings, while the dashed line through the $L = 4$ and $L = 6$ data cross at slightly higher T. Where error bars are not apparent, they are smaller than the symbol size.

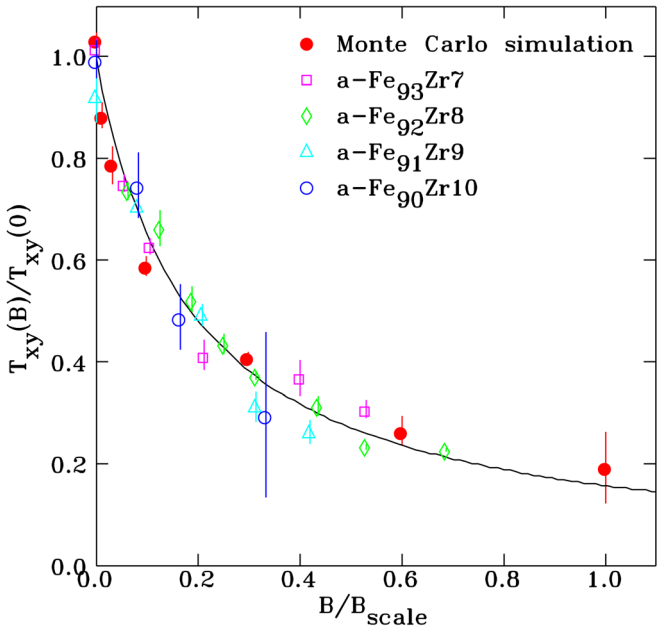

FIG. 3. (Color online) A comparison of $T_{xy}(B)$ obtained from Monte Carlo simulations with $T_{xy}(B)$ obtained from experiments on a—Fe_xZr_{100-x}. The solid line is a fit to Eq. (1).

was determined by averaging the three crossing temperatures for $L > 6$. The same range of system sizes ($L \leq 12$) yields a crossing,[7] which agrees with $L \leq 32$ (Refs. 8 and 11) in the case of the pure spin glass with Gaussian J_{ij}; similar results are expected from these calculations.[20] The crossing at T_{xy} clearly moves to lower temperatures with increasing B. As Fig. 3 clearly shows, we obtain the *same* $1/B$ scaling for $T_{xy}(B)$ in the numerical models as we did for the μSR experiments.

The scaling behavior of T_{xy} shown in Fig. 3 is remarkably consistent both across all samples, reinforcing the assertion that the $1/B$ scaling is not unique to a specific composition, and for the simulation data. In the plot, the data have been collapsed by normalizing each curve to the zero field T_{xy} value obtained from a fit to Eq. (1) and by scaling the magnetic field using $B_{scale} \sim 10$ T (except for a—$Fe_{90}Zr_{10}$, where a $B_{scale} \sim 3$ T was used — see below), such that the x and y axes of the plot are dimensionless. A simple estimate of the expected scale factor between experiment and simulation can be made by first noting that, in the model, T_{xy} drops by a factor of five from $B = 0$ to $B = 1$ (Fig. 3) and that the thermal energy/spin of the $T_{xy}(B = 0)$ state is roughly equal to the Zeeman energy of the $T_{xy}(B = 1)$ state, where the spins are almost fully aligned with the field. Equating the thermal energy at $B = 0$ in a real material ($\sim k_B T_{xy}$) to the Zeeman energy ($\sim \mu B_{scale}$) gives a simple estimate of $B_{scale} \sim 50$ T (using $T_{xy} \sim 50$ K and $\mu = 1.56\ \mu_B$[21]), demonstrating the close accord between our model and experiments.

This consistency across experiments and simulation raises the question of whether the functional form given in Eq. (1) is exact. We emphasize here that we do not believe this to be the case, but rather that Eq. (1) is likely an approximation to a more complex form. Indeed, inspection of Fig. 3 reveals that $T_{xy}(B)$ found in the simulations lies slightly below the fitted curve at small B and slightly above it at larger B. Were we to restrict the analysis to small B only, the fitted curve would be steeper than it is in Fig. 3 and would then pass well below the high field observations. Such a low-field biased fit would yield a much smaller scaling field (B_{scale}), as T_{xy} decreased more rapidly with field. Indeed, it is this very mis-fit that leads to the low scaling field noted above for a—$Fe_{90}Zr_{10}$: because of the much lower value of $T_{xy}(0)$ for $x = 90$, we could only follow $T_{xy}(B)$ as far as $B = 1$ T and not to 5.5 T, as was possible for the other materials. This limitation places us firmly in the low-field regime and yields a fit that is too steep and, thus, yields a smaller value for B_{scale}.

The consistency between experiment and simulations in both the topology of the phase diagram, the nature of the phases, and the field shift in T_{xy} is further reinforced by the *deviations* from the 1/B form for T_{xy}(B) being the same in both cases, confirming that the model captures the essential physics of the experimental system.

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