

Spin-glass ordering in diluted magnetic semiconductors: A Monte Carlo study

E. Marinari,¹ V. Martín-Mayor,¹ and A. Pagnani²

¹ *Dipartimento di Fisica, Università di Roma "La Sapienza," P. Aldo Moro 2, 00185 Roma, Italy
and INFN Sezione di Roma, INFN Unità di Roma, Roma, Italy*

² *Dipartimento di Fisica and INFN, Università di Roma "Tor Vergata," V. della Ricerca Scientifica 1, 00133 Roma, Italy
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We study the temperature-dilution phase diagram of a site-diluted Heisenberg antiferromagnet on a face-centered-cubic lattice, with and without the Dzyaloshinskii-Moriya anisotropic term, fixed to realistic microscopic parameters for IIB_{1-x}Mn_xTe (IIB=Cd,Hg,Zn). We show that the dipolar Dzyaloshinskii-Moriya anisotropy induces a finite-temperature phase transition to a spin-glass phase, at dilutions larger than 80%. The resulting probability distribution of the order parameter $P(q)$ is similar to the one found in the cubic lattice Edwards-Anderson-Ising model. The critical exponents undergo large finite-size corrections, but tend to values similar to the ones of the Edwards-Anderson-Ising model.

Although most theoretical investigations on spin-glass (SG) systems¹ have focused on models based on Ising spins, systems that have been investigated in the recent period, like the diluted magnetic semiconductors IIB Mn Te series, IIB=Cd, Hg, Zn, i.e., Cd_{1-x}Mn_xTe,^{2,3} Hg_{1-x}Mn_xTe,³ and Zn_{1-x}Mn_xTe⁴ (and somehow even typical experimental samples⁵ like CuMn, AgMn, Eu_xSr_{1-x}S), are closer in nature to continuous Heisenberg spins. Early computer simulations suggested that in three spatial dimensions neither systems with local interactions and Heisenberg⁶⁻⁸ or XY^{6,9} spins, nor systems with long-range Ruderman-Kittel (-Kasuya)-Yosida interactions¹⁰ undergo a finite-temperature SG phase transition. This fact could be potentially annoying from a phenomenological point of view, but it becomes acceptable after noticing that a small anisotropic interaction, neglected in the above calculations, could induce a finite-temperature SG phase transition.

Still the situation is not crystal clear: the work of Ref. 11 claimed that the most important anisotropic coupling in IIB Mn Te materials,¹² the Dzyaloshinskii-Moriya (DM) interaction, is not able to induce a SG phase. On the contrary a theoretical analysis¹³ of experimental data on the IIB Mn Te series was used to suggest the presence of SG ordering in three-dimensional (3D) Heisenberg spin glasses (for finite temperature and no anisotropies): recent numerical simulations¹⁴ support the existence of a chiral phase transition in such systems. The role of the anisotropy was reconsidered in Ref. 15, where the Heisenberg spin Edwards-Anderson (HEA) model was considered with the addition of a random pseudodipolar interaction: clear signatures of a finite-temperature SG phase were found. This result is not consistent with the one of Ref. 11 (that was considered as being based on a realistic modelization of IIB Mn Te, even if the direction of the DM vectors, see (1), was chosen at random, while they should be periodic along the lattice¹²). Further works on this subject can be found in Ref. 26. We remind at last that a diluted Ising antiferromagnet on a fcc lattice has been studied in Ref 16, where the signature of a SG phase transition for low enough densities has been detected.

We have taken here the point of view of trying to be as realistic as possible, analyzing a model as close as possible to the experimental samples. We show that nonrandom DM terms (selecting a realistic value for the anisotropy) are able to induce a SG phase transition in a 3D Heisenberg spin glass on a fcc lattice. We analyze and discuss in detail the values of critical exponents: the experimental results for the IIB_{1-x}Mn_xTe materials^{2,4} are in good agreement with the most accurate calculations for the Edwards-Anderson model with Ising spins (IEA) on the cubic lattice¹⁷ ($\nu = 1.8 \pm 0.2$), $\eta = -0.26 \pm 0.04$), but the numerical simulations of Ref. 16 and of Ref. 15, yielded $\nu \approx 1.0$. We will show that the numerical calculation of the critical exponents on the accessible lattice sizes suffer from serious finite-size corrections, and that a systematic analysis of the numerical data establishes a clear trend towards values of ν larger than the ones found in Refs. 15 and 16, and close to the experimental values.

The site-diluted antiferromagnetic (AFM) Heisenberg model on the fcc lattice, with and without DM anisotropy, is a model for the IIB_{1-x}Mn_xTe series, where the Mn atoms form a fcc lattice with localized (Heisenberg) spins interacting through short-range (superexchange) AFM terms, while the magnetically inert IIB atoms randomly replaces the Mn over the lattice. An AFM interaction on the fcc lattice is frustrated, and gives rise to some interesting order-disorder phenomena,¹⁸ both with Heisenberg¹⁹ and Ising spins.²⁰ The dilution disorder deletes some of the sites on the system, thus providing the random combination of frustrated and unfrustrated plaquettes, that is believed to be essential for SG ordering. The Hamiltonian of the system is

$$H = J \sum_{\langle \mathbf{x}, \mathbf{y} \rangle'} \left[\mathbf{S}_{\mathbf{x}} \cdot \mathbf{S}_{\mathbf{y}} + \frac{D}{J} \mathbf{R}_{\mathbf{x}-\mathbf{y}} \cdot (\mathbf{S}_{\mathbf{x}} \wedge \mathbf{S}_{\mathbf{y}}) \right], \quad (1)$$

where the fields $\mathbf{S} = (S_1, S_2, S_3)$, S_1, S_2 and S_3 real with $\mathbf{S}^2 = 1$, represent the spin of the Mn atoms, and $J > 0$. A lattice site is randomly occupied by a spin with probability p . The sum labeled by $\langle \mathbf{x}, \mathbf{y} \rangle'$ runs over the pairs of occupied nearest neighboring sites of the lattice. The unit-length vectors $\mathbf{R}_{\mathbf{x}-\mathbf{y}}$ specify the DM anisotropy, and they verify $\mathbf{R}_{\mathbf{x}-\mathbf{y}} = -\mathbf{R}_{\mathbf{y}-\mathbf{x}}$. Following Ref. 12 we set

$$\mathbf{R}_{(1/\sqrt{2}, 1/\sqrt{2}, 0)} = \left(\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0 \right),$$

while the other five independent vectors are obtained using the threefold rotation symmetries of the lattice. In Ref. 12 the ratio D/J has been estimated to be 0.054 for $\text{Zn}_{0.77}\text{Mn}_{0.33}\text{Te}$ and $\text{Cd}_{0.77}\text{Mn}_{0.33}\text{Te}$, and is very mildly dependent on the composition of the sample: we have fixed it to 0.06 for simplicity. As the local magnetic field acting on spin $\mathbf{S}_{\mathbf{x}}$ is [see Eq. (1)]

$$h_{\mathbf{x}} = J \sum_{\mathbf{y}, |\mathbf{x}-\mathbf{y}|=\sqrt{2}} \mathbf{S}_{\mathbf{y}} + \frac{D}{J} (\mathbf{S}_{\mathbf{y}} \wedge \mathbf{R}_{\mathbf{x},\mathbf{y}}), \quad (2)$$

it is easy to implement a heat-bath algorithm and the over-relaxed microcanonical algorithm of Ref. 19. We have found that the combination of these two updates tremendously reduces the thermalization effort. In the production runs we have performed a full-lattice heat-bath sweep followed by 19 overrelaxed updates, that will be referred in the following as an elementary Monte Carlo step (EMCS). In order to define the observables, it is useful to consider a *replica* [i.e., a thermally independent system with the same set of occupied sites, that we denote $\tilde{\mathbf{S}}(\mathbf{x})$]. The measured observables can be most easily described in terms of the following three basic fields: the tensor field [$\tau_{\alpha,\beta}(\mathbf{x}) = S_{\mathbf{x}}^{\alpha} S_{\mathbf{x}}^{\beta} - \frac{1}{3} \delta^{\alpha,\beta}$, if the lattice site \mathbf{x} is occupied, and zero otherwise], the tensorial overlap [$O_{\alpha,\beta}(\mathbf{x}) = S_{\mathbf{x}}^{\alpha} \tilde{S}_{\mathbf{x}}^{\beta}$], and the scalar overlap field [$q(\mathbf{x}) = \mathbf{S}_{\mathbf{x}} \cdot \tilde{\mathbf{S}}_{\mathbf{x}}$].

The rationale for studying the tensor field $\tau(\mathbf{x})$ ²¹ is that previous studies of AFM diluted systems on the fcc lattice,¹⁶ showed that only for moderate dilutions the system ceases to develop AFM ordering. The tensorial magnetization is an ideal order parameter to check this possibility, since it will be nonvanishing for *any* conceivable type of AFM or helical ordering. Moreover, it would also work on more sophisticated, yet trivial situations like those found in $D=0, p=1$.¹⁹ The tensorial overlap²² is most adequate to study the isotropic ($D=0$) case, since in this situation the Hamiltonian posses a $O(3)$ global symmetry: when the anisotropy is switched on the symmetry reduces to Z_2 , and the use of the scalar overlap becomes natural. For all three fields, one can define straightforwardly the corresponding susceptibility, Binder parameter, and a finite lattice correlation length.^{14,17,21}

The model (1) without impurities ($p=1.0, D=0.06J$) undergoes a phase transition at $T_c(p=1) \approx 0.60J$ from a paramagnetic phase to an AFM phase, as shown by the behavior of the tensorial magnetization. For larger dilutions a lower temperature value needs to be reached in order to exit from the paramagnetic phase: the critical line, $T_c(p)$, will eventually reach zero temperature at the percolation threshold for the magnetic ions ($p_c \approx 0.2$). The first question is for which dilution the system forgets its global AFM ordering. In order to answer this question we have performed slow annealings in 60 samples (and its corresponding replicas) at dilutions $p=1.0, 0.9$, and 0.8 , in lattices $L=8$ and 16 ; at $p=0.7$ and $p=0.6$ (that will be shown to be in the SG compositional range), we have annealed 700 samples. The results for the Binder cumulant of the tensor and scalar overlap fields at p

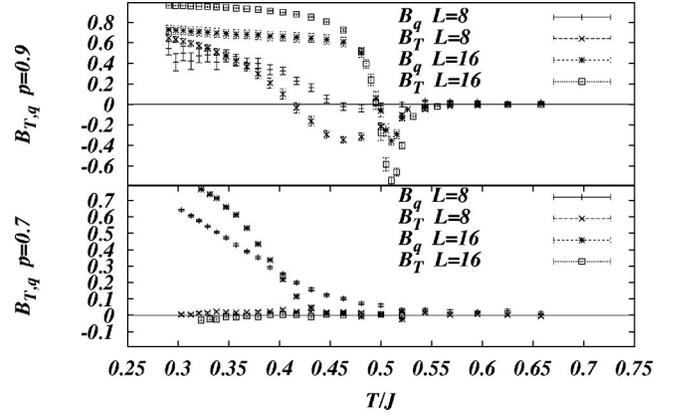


FIG. 1. Tensorial (B_T) and scalar (B_q) overlap Binder parameter versus temperature for sizes $L=8,16$ and dilution $p=0.9$ (upper part) and $p=0.7$ (lower part).

$=0.7$ and $p=0.9$ are displayed in Fig. 1. At $p=0.9$ for both observables we find a low temperature, AFM ordered phase, since the tensorial magnetization is nonvanishing. There is a strong dip close to the phase-transition point, which probably is very plausibly of first order. On the contrary for $p=0.7$, it is clear that the tensorial magnetization is no longer an appropriate order parameter. For $p=0.8$ (not shown in the plot), our results indicate a crossover regime between the two situations. Therefore, the low-temperature phase turns from AFM to SG at $0.7 < p_c < 0.8$, similar to what happens in the Ising case.¹⁶ Also for $D=0, p < 0.8$ we do not find an AFM ordered phase (see below).

In order to quantify how strong the effect of the anisotropy is, we compare the system at $p=0.7$ with $D=0$ and $D=0.06J$. In Fig. 2 we show the correlation length of the tensorial overlap in units of the lattice size. This operator should be zero in the paramagnetic phase, diverging in the SG phase, and at the critical point reaches a finite universal value. In the isotropic case (see zoom in upper part of Fig. 2) the crossing point of the $L=12$ and 16 lattices is not clearly resolved, and their respective crossings with the $L=8$ curve shifts to lower temperature with growing lattice size. In Fig. 3 we also show the Binder cumulants of the tensorial overlap and of the tensor field for $D=0$ at $p=0.7$. In addition, a long

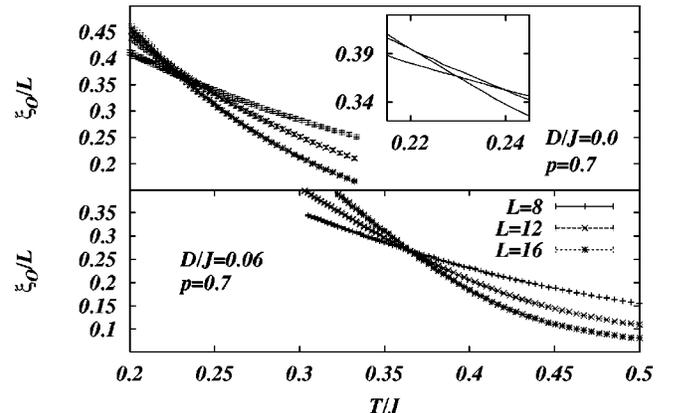


FIG. 2. Correlation length of tensorial overlap (in units of lattice size) vs temperature for $D=0$ (upper part and zoom) and in presence of anisotropy $D=0.06J$ (lower part).

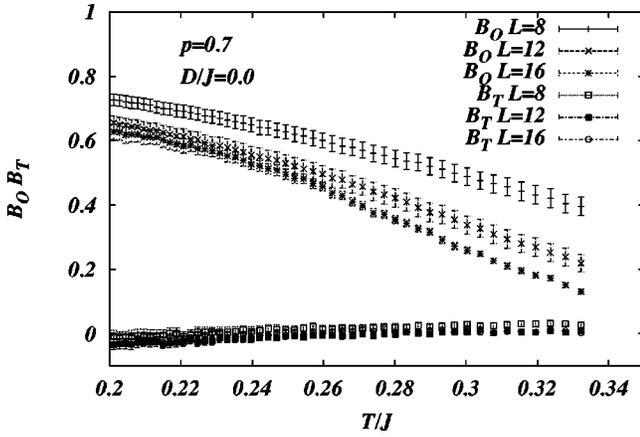


FIG. 3. Binder cumulants of the tensorial overlap and of tensor field vs temperature for $D=0$ and $p=0.7$.

run in 32 samples of size $L=32$ at $T=0.18J$ yielded a value of the Binder cumulant of the tensorial overlap of 0.30(5). From Figs. 2 and 3 it is clear that at the explored temperatures, the tensorial overlap field develops a large correlation length, while the tensor field does not, thus signaling a lack of antiferromagnetic ordering at these temperatures (of course, at still lower temperatures one cannot exclude the presence of an AFM phase). Our results are similar to the ones shown in Ref. 14 for the HEA model: the data for the Binder cumulant of the tensorial overlap rapidly grow at a certain temperature, but then saturate at a value that decreases with the lattice size (and close to the crossing temperature of the correlation length, see Figs. 2 and 3). Moreover, in Ref. 14 it has been shown that the chiral-glass phase appears precisely at the temperatures at which the Binder cumulant of the tensorial overlap grows.

On the other hand, with a 6% DM anisotropy (see the lower frame of Fig. 2), we find a neat crossing of the correlation length (the tensorial overlap Binder cumulant has a marked dip, in contrast with the scalar overlap shown in the lower frame of Fig. 1). As the phase transition for the anisotropic system occurs at a temperature 80% higher than the one close to the crossings of the $D=0$ case, that according to Ref. 14 signal a real chiral-glass phase transition, the natural conclusion is that the DM anisotropy is *not* a smooth perturbation that reveals a hidden chiral-glass ordering.

In order to characterize more precisely the SG phase we have studied the distribution of the scalar overlap at $p=0.6$, $D=0.06J$, and $T=J/4.5 \approx 0.78T_c$. At this temperature we have estimated the mean thermalization time in the $L=16$ lattice, by considering a logarithmic plot of the mean overlap susceptibility of 64 samples, as a function of MC time, starting from a random configuration, and we have found it to be of order 250 EMCS. After that we have performed a run with 800 samples, with $L=8, 12, 16$, performing 8000 EMCS on each sample, and taking a measure every 4 EMCS. We display $P(q)$ in Fig. 4: the central part is remarkably stable for growing lattice size. Therefore, on the lattice sizes that we are able to thermalize, the pattern we obtain is completely analogous to the one found for the IEA model in 3D.²³

Due to the global Z_2 symmetry of the Hamiltonian (1), one would expect it to belong to the same universality class

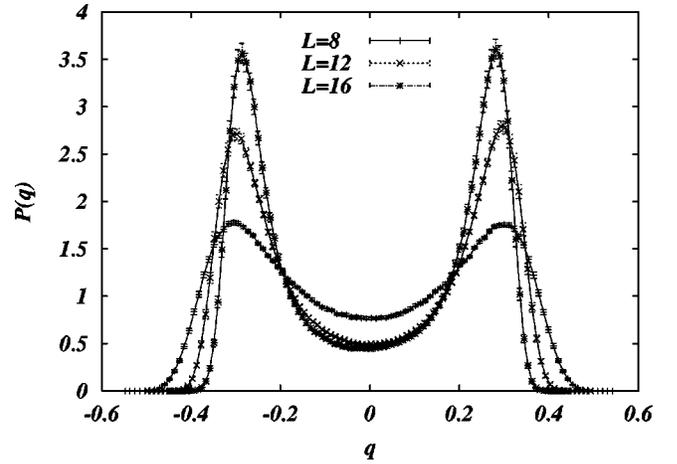


FIG. 4. Probability distribution function of scalar overlap for $L=8, 12, 16$ at $p=0.6$, $T=J/4.5 \approx 0.78T_c$ and $D=0.06J$.

of the IEA model in 3D, which seems even more plausible from our measures of the $P(q)$. To further investigate this relation we have measured the critical exponents, in the dilution range where we definitively find SG ordering, namely, $p=0.7$ and 0.6 . Since we have at our disposal only a narrow range of lattice sizes, it is important to use a finite-size scaling analysis that allows us to study the scaling corrections. We have used the quotient method of Ref. 21, that has been particularly useful in the study of scaling corrections in disordered systems.²⁴ We measure an operator O , diverging in the infinite size limit at criticality as $|T-T_c|^{-x_O}$, on two finite lattices of sides L and sL , and we select the temperature value where the two correlation lengths in units of the lattice size coincide (see the crossing of Fig. 2). For the quotient of these two measures we have

$$\frac{O(sL, T)}{O(L, T)} \Big|_{\xi(sL, T)/\xi(L, T)=s} = s^{x_O/\nu} [1 + \mathcal{O}(L^{-\omega})], \quad (3)$$

where $\omega > 0$ is related to the first irrelevant operator in the renormalization-group sense. The main advantage of the relation (3) is that the large statistical correlation between the measurements of O and ξ allows us to measure the quotient with sufficient accuracy as to uncover the scaling corrections. In our Z_2 symmetric case we have of course used the scalar overlap correlation length. Our results are displayed in Table I, and they do show the presence of significant scaling corrections (ν is computed using the temperature derivative of ξ_q , η from the susceptibility of the scalar overlap). Since we only have few lattice sizes it is meaningless to try an infinite size extrapolation as the one of Ref. 24. We should still mention that the critical exponents obtained by a simple log-log fit (for instance, with data measured at the maximum

TABLE I. Transient critical exponents $\nu(L_1, L_2)$ and $\eta(L_1, L_2)$ obtained with the quotient method (see the text).

(L_1, L_2)	$\nu(p=0.7)$	$\nu(p=0.6)$	$\eta(p=0.7)$	$\eta(p=0.6)$
(8,12)	0.941(9)	1.08(2)	0.443(6)	0.193(8)
(8,16)	1.055(13)	1.32(2)	0.392(3)	0.0959(12)
(12,16)	1.277(22)	1.91(7)	0.28(6)	-0.10(5)

of the specific heat) is roughly equivalent to an average of the transient exponents displayed in our table. Therefore the value of $\nu \approx 1$ found with Ising spins¹⁶ or in the HEA model with pseudodipolar anisotropy,¹⁵ is most probably a preasymptotic value. In fact, the best available results for the IEA model in 3D Ref. 17, $\nu = 1.8(2)$, $\eta = -0.26(4)$ are plausible infinite volume extrapolations for our results. However, in order to definitively elucidate this point, it would be helpful to use the extrapolation method of Refs. 17 and 25, that allows us to work in the paramagnetic region with a significantly smaller thermalization effort.

We have shown for the first time that dipolar DM anisotropic local interactions are able to induce a SG phase transition for Heisenberg spins in three dimensions. This result has been obtained with the very small realistic value of the anisotropy coupling constant in the IIB Mn Te series. Given the dramatic effect of this small perturbation term in the Hamiltonian, we suggest that the chiral-glass mechanism proposed in Ref. 13 is overwhelmed by the neglected DM term. We have studied the temperature-dilution phase diagram of the Hamiltonian (1) in a large dilution range. We have found that the low-temperature phase changes from AFM to SG order between $p = 0.8$ and $p = 0.7$. We have used

a combination of microcanonical and heat-bath Monte Carlo update, that have allowed us to thermalize a $L = 16$ lattice at $T = 0.78T_c$, in the SG phase. We have measured the distribution of the overlap, finding results analogous to the ones of an IEA 3D model on similar lattice sizes. We have given an estimate the critical exponents on the SG dilution range. Our results suffer from severe finite-size corrections, but it is plausible to deduce that critical exponents are converging to the IEA results, as the experimental results for the IIB Mn Te suggest.^{2,4} Further open questions need clarification: a better measure of the critical exponents using the method of Ref. 25, the precise characterization of the AFM phase, and a detailed study of the order of the paramagnetic antiferromagnetic phase transition at low dilution.

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