Spin Glass Ordering in Diluted Magnetic Semiconductors: a Monte Carlo Study

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We study the temperature-dilution phase diagram of a site-diluted Heisenberg anti-ferromagnet on a fcc 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.

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Although most theoretical investigations on spin glass (SG) systems have focused on models based on Ising spins, systems that have been investigated in the recent period, like the diluted magnetic semiconductors $IIB_{1-x}Mn_xTe$ series, $IIB = Cd, Hg, Zn$, i.e. $Cd_{1-x}Mn_xTe$ (\textsuperscript{18}), $Hg_{1-x}Mn_xTe$ (\textsuperscript{3}) and $Zn_{1-x}Mn_xTe$ (\textsuperscript{3}) (and somehow even typical experimental samples like CuMn, AgMn, Eu$_x$Sr$_{1-x}$S), are closer in nature to continuous Heisenberg spins. Early computer simulations suggested that in three spatial dimensions neither systems with local interactions and Heisenberg or XY spins, nor systems with long-range RKKY interactions 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 \textsuperscript{11} claimed that the most important anisotropic coupling in $IIB_{1-x}Mn_xTe$ materials \textsuperscript{13}, the Dzyaloshinskii-Moriya (DM) interaction, is not able to induce a SG phase. On the contrary a theoretical analysis \textsuperscript{13} of experimental data on the $IIB_{1-x}Mn_xTe$ series was used to suggest the presence of SG ordering in 3D Heisenberg spin glasses (for finite temperature and no anisotropies): recent numerical simulations \textsuperscript{14} support the existence of a chiral phase transition in such systems. The role of the anisotropy was reconsidered in \textsuperscript{14}, where the Heisenberg spin Edwards-Anderson (HEA) model was considered with the addition of a random pseudo-dipolar interaction: clear signatures of a finite temperature SG phase were found. This result is not consistent with the one of \textsuperscript{11} (that was considered as being based on a realistic modelization of $IIB_{1-x}Mn_xTe$, even if the direction of the DM vectors, see \textsuperscript{12}, was chosen at random, while they should be periodic along the lattice\textsuperscript{12}). We remind at last that a diluted Ising anti-ferromagnet on a fcc lattice has been studied in \textsuperscript{17}, 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 non-random 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 \textsuperscript{14} are in good agreement with the most accurate calculations for the Edwards-Anderson model with Ising spins (IEA) on the cubic lattice \textsuperscript{17} ($\nu = 1.8 \pm 0.2, \eta = -0.26 \pm 0.04$), but the numerical simulations of \textsuperscript{13} and of \textsuperscript{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 clear trend towards values of $\nu$ larger than the ones found in \textsuperscript{13,16}, and close to the experimental values.

The site-diluted anti-ferromagnetic (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 an fcc lattice with localized (Heisenberg) spins interacting through short-range (super-exchange) 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 \textsuperscript{18}, both with Heisenberg \textsuperscript{19} and Ising spins \textsuperscript{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
where the fields $S = (S_1, S_2, S_3)$, $S_1$, $S_2$ and $S_3$ real with $S^2 = 1$, 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 $(x,y)$ runs over the pairs of occupied nearest neighboring sites of the lattice. The unit-length vectors $R_{x-y}$ specify the DM anisotropy, and they verify $R_{x-y} = -R_{y-x}$. Following \[2\] we set $R_{(\frac{\sqrt{2}}{2},\frac{\sqrt{2}}{2})} = (\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0)$, while the other five independent vectors are obtained using the three-fold rotation symmetries of the lattice. In Ref. \[13\] the ratio $D/J$ has been estimated to be 0.054 for $Zn_{77}Mn_{33}Te$ and $Cd_{77}Mn_{33}Te$, 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 $S_x$ is (see \[1\])

$$H = J \sum_{(x,y)} \left[ S_x \cdot S_y + \frac{D}{J} R_{x-y} \cdot (S_x \wedge S_y) \right],$$

it is easy to implement a heat-bath algorithm and the over-relaxed micro-canonical algorithm of \[19\]. 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 over-relaxed 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 $\tilde{S}(x)$). The measured observables can be most easily described in terms of the following three basic fields: the tensor field $(\tau_{\alpha,\beta}(x) = S_\alpha S_\beta - \frac{1}{2} \delta_{\alpha,\beta}$, if the lattice site $x$ is occupied, and zero otherwise), the tensorial overlap $(O_{\alpha,\beta}(x) = S_\alpha \tilde{S}_\beta)$, and the scalar overlap field $(q(x) = S_x \cdot \tilde{S}_x)$.

The rationale for studying the tensor field $\tau(x)$ \[21\] 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 non-vanishing for any conceivable type of AFM or helicoidal ordering. Moreover, it would also work on more sophisticated, yet trivial situations like the found in $D = 0, p = 1$ \[19\]. The tensorial overlap \[22\] 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 \[14,17,21\].

![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).](image)
their respective crossings with the $L = 8$ curve shifts to lower temperature with growing lattice size. Moreover, the data (not shown in the plot) for the Binder Cumulant of the tensorial overlap rapidly grow at the crossing temperature of the correlation length, but then saturate at a value which decreases with the lattice size, without a crossing, similarly to the results shown in [14], where it has been shown that the chiral-glass phase appears precisely at the temperatures at which the Binder cumulant of the tensorial overlap grows.

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 figure 3 is 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 Ising EA model in 3D [24].

Due to the global $Z_2$ symmetry of the Hamiltonian of [4], one would expect it to belong to the same universality class 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 to study the scaling corrections. We have used the quotient method of [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 $|T - T_c|^{-\xi O}$, 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 figure 2). For the quotient of these two measures we have

$$
\frac{O(L, T)}{O(sL, T)} = s^{\xi O/\nu} (1 + O(L^{-\omega})) ,
$$

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 $\xi$ allows 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 3 and they do show the presence of significant scaling corrections ($\nu$ is computed using the temperature derivative of $\xi D$, $\eta$ 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 [24]. We should still mention that the critical exponents obtained by a simple log-log fit (for instance, with data measured at the maximum 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 spins [10] or in the HEA model with pseudo-dipolar anisotropy in [14] is most probably a preasymptotic value. In fact, the best available results for the IEA model in 3D [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 [25,17], that allows 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 IIIB Mn Te series. Given the dramatic effect of this small perturbation term in the Hamiltonian, we suggest that the chiral-glass mechanism proposed in [13] is overwhelmed by the neglected DM term. We have studied the temperature-dilution phase diagram of the Hamiltonian 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 micro-canonical 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 Ising EA 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 Ising EA results, as the experimental results for the IIIB Mn Te suggest [24]. Further open questions need clarification: a better measure of the critical exponents using the method of [23], the precise characterization of the AFM phase, and a detailed study of the order of the paramagnetic anti-ferromagnetic phase transition at low dilution.

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| $(L_1, L_2)$ | $\nu(p = 0.7)$ | $\nu(p = 0.6)$ | $\eta(p = 0.7)$ | $\eta(p = 0.6)$ |
|--------------|----------------|----------------|----------------|----------------|
| (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)       |

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

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