Exchange anisotropy, disorder and frustration in diluted, predominantly ferromagnetic, Heisenberg spin systems

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Motivated by the recent suggestion of anisotropic effective exchange interactions between Mn spins in Ga$_{1-x}$Mn$_x$As (arising as a result of spin-orbit coupling), we study their effects in diluted Heisenberg spin systems. We perform Monte Carlo simulations on several phenomenological model spin Hamiltonians, and investigate the extent to which frustration induced by anisotropic exchanges can reduce the low temperature magnetization in these models and the interplay of this effect with disorder in the exchange. In a model with low coordination number and purely ferromagnetic (FM) exchanges, we find that the low temperature magnetization is gradually reduced as exchange anisotropy is turned on. However, as the connectivity of the model is increased, the effect of small-to-moderate anisotropy is suppressed, and the magnetization regains its maximum saturation value at low temperatures unless the distribution of exchanges is very wide. To obtain significant suppression of the low temperature magnetization in a model with high connectivity, as is found for long-range interactions, we find it necessary to have both ferromagnetic and antiferromagnetic (AFM) exchanges (e.g. as in the RKKY interaction). This implies that disorder in the sign of the exchange interaction is much more effective in suppressing magnetization at low temperatures than exchange anisotropy.

I. INTRODUCTION

It has recently been suggested that frustration effects may be important for the magnetic properties of diluted magnetic semiconductors (DMSs) such as Ga$_{1-x}$Mn$_x$As. The reported Curie temperatures ($T_C$) in these compounds continue to rise, with a maximum of 140K recently reported for Ga$_{1-x}$Mn$_x$As with even higher temperatures reported for related materials. Aside from increasing $T_C$, it will also be important to have a thorough understanding of the different aspects of their magnetic properties over a wide temperature range in order to be able to construct optimized spintronic devices. In theoretical analyses, Zarand and Janko showed that within the RKKY approximation, a proper treatment of the spin-orbit coupling leads to anisotropic exchanges between Mn spins. Using this interaction they found that the saturation magnetization is reduced by up to 50% at low temperatures. Experimentally it has been observed that in many DMS, the saturation magnetization at low temperatures is not as large as would be expected if all Mn moments were aligned (i.e. the full saturation value). While it is likely that magnetically inactive Mn, such as Mn interstitials may account for some of the suppression of the low-temperature magnetization, the results of Zarand and Janko suggest that anisotropic spin interactions may also play a significant role in accounting for it. We carefully investigate this possibility in this paper.

In a system consisting of localized spins (local moments) coupled to non-interacting fermions (carriers), where the spin-carrier interaction is a perturbation on the fermion Hamiltonian, the low-lying spin excitations can be described in terms of an RKKY interaction between the spins. In the case of DMS, the carrier density is low (in fact, lower than the density of local moments by a considerable factor, due to carrier compensation), and the carrier-spin interaction is quite strong (necessary to enable a high $T_C$). Consequently, the RKKY approximation appears unlikely to be appropriate for a quantitative description of the ferromagnetism in Ga$_{1-x}$Mn$_x$As since the Fermi energy is not necessarily much larger than the magnetic coupling. However, the qualitative prediction of anisotropic exchange may be present in more precise treatments.

In what follows, therefore, we assume that the magnetic properties of the system can be modeled in terms of an effective spin Hamiltonian, with a form that maintains the symmetry properties of the RKKY interactions obtained in the weak-coupling limit. Rather than calculate the anisotropy in the Mn-Mn effective exchange within a microscopic model, we use a different approach to investigate the relevance of anisotropy for systems of diluted spins. We consider phenomenological models with disordered, anisotropic exchanges between classical Heisenberg spins placed randomly at low densities on a fcc lattice (corresponding to the Ga fcc sublattice in (Ga,Mn)As), and study the magnetic properties for several functional forms of the exchange interactions. In each case we consider various values of the disorder and
anisotropy. We focus on whether full saturation in magnetization is reached at low temperatures and also investigate the magnetic susceptibility, since this is known to be a good experimental indicator of spin freezing. Our results allow us to infer parameter ranges in which anisotropy and/or disorder are likely to play an important role in the magnetic properties of such systems.

The paper is organized as follows: in Sec. II we describe the models we study and how disorder and anisotropy are incorporated into each of them. Section III lists the quantities we calculate and how we perform the Monte Carlo simulations. Section IV shows our results for the magnetization, susceptibility and Curie temperature and finally in Sec. V we discuss our results and their implications for modeling III-V DMS.

II. MODEL

We consider \( N_d \) spins randomly distributed at locations \( \mathbf{R}_i, \) \( i = 1, \ldots, N_d \) on a fcc lattice of size \( N \times N \times N \), corresponding to an impurity concentration \( x = N_d/4N^3 \). The spins are treated as classical variables (Mn spins in Ga\(_{1-\varepsilon}\)Mn\(_\varepsilon\)As have \( S = \frac{5}{2} \), so this is a reasonable approximation). For simplicity, we take the classical spins to have unit length; this is equivalent to rescaling the exchange from \( J \) to \( JS^2 \), i.e. changing the units of energy. The most general formulation of the problem we consider in this study is provided by the Heisenberg Hamiltonian

\[
\mathcal{H} = -\sum_{i,j} \sum_{\alpha\beta} J_{ij} F_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j) S_i^\alpha S_j^\beta,
\]

where \( \alpha \) and \( \beta \) index Cartesian coordinates. The exchange coupling \( J_{ij} F_{\alpha\beta} \) is written as a product of a random variable \( J_{ij} \), and a function \( F \) of the separation of the two spins, for reasons that will become clear later. Since the sites are not on a regular lattice, the summation over site index is always over all sites of the system. For uncoupled spins \( i \) and \( j \) we simply have \( F_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j) = 0 \).

We consider the exchange integral to be parameterized as:

\[
F_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j) = \left( \lambda \delta_{\alpha\beta} + (1 - \lambda) \hat{e}_{ij}^\alpha \hat{e}_{ij}^\beta \right) f(r),
\]

where \( r = |\mathbf{R}_i - \mathbf{R}_j| \) and the unit vector \( \hat{e}_{ij} = (\mathbf{R}_i - \mathbf{R}_j)/|\mathbf{R}_i - \mathbf{R}_j| \). The parameter \( \lambda \) controls the exchange anisotropy, where \( \hat{e}_{ij} \) defines the axis of anisotropy for the pair of spins \( S_i \) and \( S_j \) located at positions \( \mathbf{R}_i \) and \( \mathbf{R}_j \). Using Eq. (2), the effective interaction can now be rewritten as \( J_{ij} S_i^\alpha F_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j) S_j^\beta = J_{ij} f(r) \left( S_i^\alpha S_j^\beta + \lambda S_i^\| S_j^\| + \lambda S_i^\perp S_j^\perp \right) \), where the parallel and perpendicular components are defined with respect to \( \hat{e}_{ij} \). As a result, for \( \lambda = 1 \) the model has no anisotropy and reduces to a simple disordered Heisenberg model. For \( 0 < \lambda < 1 \) the couplings become anisotropic and favor alignment of each pair of spins along their positional axis \( \hat{e}_{ij} \), whilst for \( \lambda > 1 \), the couplings favor alignment perpendicular to this axis (see Fig. I). Since the relevant directions \( \hat{e}_{ij} \) differ considerably from pair to pair, some frustration is introduced into the system, possibly leading to spin-glass physics.

The function \( f(r) \) describes the spatial variation of the exchange interactions. In this work we investigate the following possibilities:

\[
f(r) = \begin{cases} 
\theta(R - r) & \text{Short range FM, model A,} \\
\frac{\sin y - y \cos y}{y^4} & \text{RKKY, model B,} \\
\frac{1}{r^4} & \text{Long range FM, model C,}
\end{cases}
\]

where \( y = 2k_Fr \), and \( k_F \) is the Fermi wavevector. In the short range model, equal-strength ferromagnetic interactions exist only between neighboring spins within distance \( R_c \) of one another. The RKKY model allows interactions between all spins in the system, with oscillating sign depending on the Fermi wave-vector \( k_F \) corresponding to different carrier concentrations. Finally we consider a purely ferromagnetic model with long-range (power-law) interaction. A comparison between the short-range and the long-range models clarifies the role played by the range of the exchange, while a comparison between the RKKY and the long-range model clarifies the importance of the exchange sign oscillations.

In the RKKY approach of Zarand and Janko, the relative magnitudes of the exchanges parallel and perpendicular to the line joining two Mn spins, \( K_{\parallel}(r) \) and \( K_{\perp}(r) \) respectively, depend on the distance \( r \) between the two spins. As a rough guide to compare with the models we use in this work, \( |K_{\perp}(r)| > |K_{\parallel}(r)| \) for large \( r \) while \( |K_{\parallel}(r)| > |K_{\perp}(r)| \) for small \( r \). It should be noted that we use the RKKY interaction for illustrative purposes only, since the exchange interactions in a more realistic model of DMS will likely be quantitatively different.

![Fig. 1: Schematic representation of the two different types of anisotropy parametrized by \( \lambda \). If \( \lambda > 1 \), the anisotropy defines an easy plane for the interactions between two spins, whilst if \( \lambda < 1 \) the anisotropy defines an easy axis.](image-url)
As demonstrated in mean-field and Monte Carlo studies of an impurity band model for III-V diluted magnetic semiconductors and in studies of the kinetic-exchange model of III-V DMS including disorder and Coulomb interactions of the charge carrier with the Mn acceptors, inhomogeneity induced by positional disorder of the Mn spins implies different local carrier charge densities at different sites, which in turn leads to a broad distribution of effective local fields created at various Mn sites by the itinerant carriers. If one integrates out the fermionic degrees of freedom and formulates the problem in terms of effective exchanges between the Mn spins, there should also be a wide distribution of their effective exchanges. To incorporate the effect of positional disorder leading to a wide distribution of magnitudes of the exchanges in our model, we assume that \( J_{ij} = \epsilon_i \epsilon_j \), where the \( \epsilon_i \) are random variables attached to each site, such that their logarithm \( z_i = \log_{10} \epsilon_i \) has a Gaussian distribution

\[
P_{n_i}(z_i) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left[ -\frac{(z_i - z(n_i))^2}{2\sigma^2} \right],
\]

although the precise form of the disorder should not change our conclusions. In Eq. (4), the mean value of \( z_i, z(n_i) \) is taken to depend on the number of nearest neighbors spins (i.e., within a distance \( R_c \)) of the site \( i \), \( n_i \) though the relation \( z(n_i) = \sigma(n_i - n_0) \), where \( n_0 \) is the average number of neighbors for a given cutoff \( R_c \). In our simulations \( R_c \) is chosen such that \( n_0 = 6 \) or 12.

This scheme naturally favors stronger couplings within more dense clusters (higher \( n_i \) values) and hence should mimic some of the phenomenology observed in the impurity band model for III-V DMS, where holes congregate in regions of higher Mn density and therefore lead to stronger effective interactions between the Mn in these regions. The parameter \( \sigma \) controls the width of the distribution of couplings, and therefore we use it to characterize the disorder present in the system; a more disordered system with a wider distribution of couplings corresponds to a larger value of \( \sigma \).

Thus, the three parameters that control the behavior of the model are: (i) \( \lambda \), which controls the amount of anisotropy; (ii) \( \sigma \), which controls the disorder-induced width of the distribution of effective exchanges, and (iii) \( R_c \), which defines the average number of nearest neighbors for the short range model (for the RKKY and long range models, \( R_c = \infty \)).

III. SIMULATIONS

We have performed exhaustive Monte Carlo simulations on each of models A, B and C for temperatures above the ordering temperature \( T_c \) to well below \( T_c \). We use a range of sizes to determine \( T_c \) via finite size scaling, and average over a sufficient number of realizations of the disordered systems for each size to determine average quantities.

A. Parameters and calculated quantities

We investigated systems of linear sizes \( L = 11, 14 \) and 17, containing \( N_d = 53, 110 \) and 196 spins respectively. This corresponds to a Mn density in Ga\(_{1-x}\)Mn\(_x\)As of \( x = 0.01 \). The interaction range \( R_c \) is chosen such that the average number of nearest neighbors within \( R_c \) is either \( n_0 = 6 \), or \( n_0 = 12 \). We studied the short range model for both values of \( n_0 \). Note that for models with short-range interactions, the value of \( x \) has no qualitative effect on the behavior of magnetic properties for \( x \leq 0.05 \), since changing the concentration is equivalent to a pure rescaling of all inter-spin distances by a fixed factor. The value of \( x \) becomes relevant for larger concentrations, where the average inter-spin distance is comparable with the lattice constant. The anisotropy values considered were in the range \( \lambda = 0.1 \) to \( \lambda = 10 \), with the isotropic case \( \lambda = 1 \) used as a reference.

For the short range model, two different disorder values were considered for most anisotropy values, whilst for the other models, only one disorder strength was considered. The values of \( \sigma \) considered were: in the short range model, \( \sigma = 0.017 \) and 0.05 for \( n_0 = 6 \), and \( \sigma = 0.01 \) and 0.03 for \( n_0 = 12 \). In the long range model we chose \( \sigma = 0.03 \), while for the RKKY model, \( \sigma = 0.01 \). These values were chosen such that meaningful comparisons between different models can be performed, subject to some computational constraints. Figure 2 shows the actual distribution of \( J_{ij} \) used in the simulation for two different values of \( \sigma \).

![FIG. 2: Distribution of log\(_{10} J_{ij} \). Each curve is an average of 5 samples with \( L = 32 \), \( N_d = 1310 \) and \( n_0 = 6 \). The distribution is almost Gaussian, and its width increases with increasing \( \sigma \).](image)
ages for the following quantities: (i) the magnetization

\[ M = \left\langle \frac{1}{N_d} \left| \sum_i S_i \right| \right\rangle, \tag{5} \]

and (ii) the magnetic linear susceptibility

\[ \chi_m = \beta \left( \frac{1}{N_d} \left| \sum_i S_i \right|^2 - M^2 \right). \tag{6} \]

To determine the Curie temperature in our samples we calculated the Binder cumulant

\[ G(L, T) = \frac{1}{2} \left( 5 - 3 \left\langle \frac{1}{N_d} \left| \sum_i S_i \right|^4 \right\rangle \right) \tag{7} \]

and used finite size scaling. \( G(L, T) \) is defined such that in the paramagnetic phase it decreases with \( L \), and tends to zero as \( L \to \infty \), while in the ferromagnetic phase it increases with increasing size \( L \) and tends to unity in the thermodynamic limit. Near the transition temperature \( T_c \), this dimensionless quantity has the finite size scaling form \( G(L, T) = G(L^\nu(T - T_c)) \) where \( \nu \) is the exponent of the diverging spin-spin correlation length \( \xi \sim (T - T_c)^{-\nu/2}. \) Consequently, at \( T_c \), \( G(L, T_c) \) is independent of \( L \); \( T_c \) can be identified by a simultaneous crossing of \( G(L, T) \) vs. \( T \) curves for different \( L \). This method is found to be more reliable in determining \( T_c \) than the onset of magnetization, or the position of peaks in the magnetic susceptibility in relatively small finite size samples.\(^{25}\)

### B. Temperature Rescaling

In order to compare temperature scales for different \( \lambda \) values, we note that the exchange felt for a spin orientation at angle \( \theta \) to the axis \( e_{ij} \) is \( J(\theta) = J_0 \sqrt{\cos^2 \theta + \lambda^2 \sin^2 \theta} \). Thus, \( \left\langle J \right\rangle = \frac{1}{4\pi} \int d\Omega J(\theta) \) gives the average exchange integrated over all solid angles \( \Omega \). Evaluating the integral gives\(^{25}\)

\[ \left\langle J \right\rangle = J_0 \times \begin{cases} \frac{1}{2} \left[ 1 + \frac{\lambda^2}{\lambda^2 - 1} \sin^{-1} \left( \frac{\sqrt{\lambda^2 - 1}}{\lambda} \right) \right], & \lambda > 1, \\ 1, & \lambda = 1, \\ \frac{1}{\lambda^2} \left[ 1 + \frac{\lambda^2}{\sqrt{1 - \lambda^2}} \sinh^{-1} \left( \frac{\lambda}{\sqrt{1 - \lambda^2}} \right) \right], & \lambda < 1. \end{cases} \]

These factors are used to rescale the temperature for each value of \( \lambda \) chosen. The plots are for the temperature scaled as \( T/J_{\text{eff}}(\lambda) \), where \( J_{\text{eff}}(1) = J_0, J_{\text{eff}}(0.1) = 0.5150 J_0, J_{\text{eff}}(0.5) = 0.6901 J_0, J_{\text{eff}}(1.5) = 1.3463 J_0 \) and \( J_{\text{eff}}(10) = 7.8902 J_0 \).

### C. Monte Carlo Technique

The Metropolis algorithm necessitates long equilibration times at low temperatures and large values of anisotropy, due to its relatively slow sampling of phase space. As a result, we used a different method to perform spin flips. This method is formally equivalent to the Metropolis algorithm and can be used for any Hamiltonian, \( H \), involving classical spins that can be written in the form \( H = \sum_i \mathbf{h}_i \cdot \mathbf{S}_i \), where \( \mathbf{h}_i = \sum_j J_{ij} \mathbf{S}_j \) is the local field created at site \( i \) by the other spins. In our model, it also contains terms of the form \( \sum_j J_{ij} e_{ij}(\mathbf{e}_{ij} \cdot \mathbf{S}_j) \).

The implementation of a Monte Carlo simulation requires successive spin flips at each site in the system for a Monte Carlo step. Each spin flip involves changing the angular position vector of one spin, whilst keeping all others fixed. After a sufficiently large number of spin flips at each site, the angular distribution of these vectors will be equal to the equilibrium (Boltzmann) distribution. For any spin that is about to be flipped, the distribution of the angle \( \theta \) between the spin and its local field \( \mathbf{h}_i \) (integrated over azimuthal angle) is

\[ \rho(\theta) = \frac{k e^{k \cos \theta \sin \theta}}{e^k - e^{-k}}, \tag{8} \]

where \( k = \beta |\mathbf{h}_i| \). This distribution is easily integrated over \( \theta \), and hence by finding a function \( f(x) \) which maps \( x \in [0, 1] \) to \( \cos \theta \in [-1, 1] \), uniform sampling of the \( 0, 1 \) interval will give the desired distribution of \( \cos \theta \in [-1, 1] \). It is simple to find that \( f(x) \) is given by

\[ f^{-1}(\cos \theta) = x = \int_0^\theta \rho(\theta')d\theta', \tag{9} \]

and the explicit expression for this mapping is:

\[ \cos \theta = f(x) = 1 + \frac{1}{k} \ln[1 - x(1 - e^{-2k})]. \tag{10} \]

This approach is similar to those that are sometimes used in lattice field theories.\(^{25}\) We have tested that our method yields results for equilibrium quantities that are identical to the Metropolis algorithm, at the same time, the equilibration and auto-correlation times were found to be shorter by a factor from 10 to 100 depending on temperature and size when using this method for the above models for our range of \( T \) and \( L \).

If the new orientation of the spin \( \theta \) is generated in this way, each trial move is accepted, since the mapping we have made is one that changes the probability of a configuration being accepted from the Boltzmann weight to unity, provided the configuration is chosen in the prescribed manner. The calculation of the mapping function may be more time-consuming than calculation of the energy difference between initial and final states performed in the Metropolis algorithm, but it has the advantage of a 100% acceptance rate. This compares to the Metropolis algorithm which may have exponentially low acceptance.
rates. The evaluation of the mapping function can be optimized to further increase the efficiency. The calculation of $k$ takes about the same amount of time as evaluating the energy difference in the usual implementation of the Metropolis algorithm. After updating $\cos \theta$ all that remains is to generate a random azimuthal orientation of the spin by randomly selecting a vector (of appropriate magnitude) perpendicular to the local field; this can be done with a fast algorithm.

In summary, the algorithm used is: 1) compute the local field $\mathbf{h}_i$ and $k = \beta |\mathbf{h}_i|$; 2) choose a random number $x \in [0, 1]$ and use Eq. (10) to generate the new orientation $\cos \theta$; 3) update the energy; 4) generate a random azimuthal component to the spin; 5) update spin components; 6) repeat for the next spin.

We have compared this algorithm with the Metropolis algorithm for our models. They generate the same equilibrium results, however this algorithm equilibrates much faster when the model has large anisotropy and frustration. Figure 3 shows an example in which the algorithm we used reached equilibrium an order of magnitude faster than the Metropolis algorithm.

IV. RESULTS

We present the results we obtained for the magnetization for all three models. For the short range model, we also present the susceptibility and the Curie temperature.

A. Short range model

1. Magnetization

The magnetization curves $M(T)$ shown in Fig. 4 for size corresponding to $N_d = 196$ spins have the characteristic linear decrease with temperature seen in previous work and in experiments in Ga$_{1-x}$Mn$_x$As.$^{26,27}$ It is also apparent from comparing Fig. 4(a) with Fig. 4(b) that increasing the number of nearest neighbors in the short range model does not qualitatively change the shape of the magnetization curve.

With temperatures properly rescaled by $J_{\text{eff}}$, we observed that curves corresponding to the same disorder value $\sigma$ but various anisotropies $\lambda$ are almost identical at high temperatures. Increasing the disorder $\sigma$ leads to increased magnetization at high temperatures, as expected from studies of other models for DMS.$^{13,14,15}$

Anisotropy plays a role at low temperatures, where increased anisotropy does lower the $T = 0$ magnetization, although the effect is rather small. The suppression is more pronounced for $\lambda < 1$ (easy-axis) than $\lambda > 1$ (easy-plane). For $n_0 = 6$, the value of the saturation magnetization seems to depend only on $\lambda$ and be independent of $\sigma$. Whereas at higher temperatures ($T \geq 0.5 T_c$), as stated above the opposite is true. Consequently, both anisotropy and disorder in the magnitude of the ferromagnetic exchanges affect $M(T)$ in the temperature range $T = 0.1 T_c \sim 0.5 T_c$. For $n_0 = 12$, the suppression of low-temperature magnetization by anisotropy is not observed except for an extremely large anisotropy $\lambda = 0.1$.

2. Susceptibility

The behavior of the linear susceptibility for the short range model with both 6 and 12 nearest neighbors is shown in Fig. 5. After temperature rescaling, the high-temperature tails of the curves with the same $\sigma$ value are again identical. At low temperatures, anisotropy leads to a finite value for the $T = 0$ linear susceptibility. The finite value of the linear susceptibility at $T = 0$ is consistent with the incomplete saturation of magnetization in the presence of anisotropy. This effect is most transparent in the case of $n_0 = 6$; in contrast, for $n_0 = 12$, the effect of anisotropy is very weak unless the anisotropy is extreme, e.g. $\lambda > 5$ or $\lambda < 0.1$.

3. Curie Temperature

The Curie temperatures are deduced from the Binder cumulant Eq. (7) curves. Figure 6 shows curves calculated for different system sizes from the 12 neighbor model which intersect at the same temperature for a given $\lambda$, indicating the position of $T_c$. These critical
temperatures are very close to the peaks in linear susceptibility of the same model, and are tabulated in Table I. Note that the temperature is not rescaled by $J_{eff}$ in Fig. 6 in order to give a clear view of each set of curves. When the temperature is rescaled, the values of $T_c$ are approximately the same.

We conclude that small-to-moderate anisotropy has a rather small effect on the magnetic properties of the short-range model. Significant deviations from the isotropic behavior are seen only for very large values of the anisotropy, and are generally more pronounced in the $n_0 = 6$ model.

### B. Long range model

The qualitative behavior of the low-temperature magnetization in the long range model is very similar to that observed in the short range model, as can be seen in Fig. 4. Increasing the length-scale of the exchange does very little to increase the amount of frustration in the model, and in both the short-range and the long-range model the suppression of the low temperature magnetization is less than 20%, and often much smaller, for all values of anisotropy considered. This is small compared to the 50-60% reduction observed experimentally, hence other sources of frustration must be present to account for the greatly reduced low temperature magnetization as compared to that of an aligned ferromagnet. One candi-

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**TABLE I: Critical temperatures (in units of $J_{eff}$, see text) estimated from Binder cumulant $G(N,T)$ and magnetic susceptibility $\chi_M$ for $\sigma = 0.01$ and $n_0 = 12$.**

| $T_c/J_{eff}$ | $\lambda = 0.5$ | $\lambda = 1$ | $\lambda = 1.5$ |
|--------------|-----------------|----------------|-----------------|
| From $\chi_M$ | 3.42            | 3.61           | 3.50            |
| From $G(N,T)$ | 3.39            | 3.48           | 3.39            |

FIG. 4: Magnetization for (a) $n_0 = 6$ and (b) $n_0 = 12$, for various values of $\lambda$ and $\sigma$. The simulations are for $N_d = 196$ spins. The insets amplify the low temperature regions.

FIG. 5: Magnetic susceptibility for (a) $n_0 = 12$, and (b) $n_0 = 6$, with various values of $\lambda$ and $\sigma$. The simulations are for $N_d = 196$ spins.
FIG. 6: Binder cumulant for models with 12 neighbors on average, $G(N,T)$, at various anisotropy $\lambda$ and sizes $L$.

date for the source of further reduction is the antiferromagnetic component of effective Mn-Mn interactions as is found for RKKY interactions.

FIG. 7: Magnetization for $n_0 = 6$, various $\lambda$, $\sigma = 0.03$, long range model. In this case all pairs of spins interact, and $n_0$ is used only to adjust the average coupling constant.

C. RKKY models

Figure 8 shows the magnetization calculated for isotropic RKKY models with different Fermi wavelengths, corresponding to different charge carrier concentrations. The main observation is that the antiferromagnetic exchange at long distances introduced by the RKKY model has a significant effect on lowering the low temperature magnetization; the decrease is considerably larger than that due to anisotropy in purely ferromagnetic exchange interactions in the short- and long-range models considered previously.

In Fig. 8 we show curves corresponding to several different values of the Mn concentration $x$ and charge carrier compensation $1 - p$; the resulting charge carrier concentration is $n_h = 4xp/a^3$, where $a = 5.65$ Å is the GaAs lattice constant. Note that the temperature also needs to be rescaled by a factor of $(px)^{3/4}$ in 3 dimensions for RKKY interactions, to compare different magnetization curves. One interesting observation of the series with $x = 0.05$ is that increasing the hole concentration $px$ with fixed $x$ does not appear to change $T_c$ but the low temperature magnetization has a minimum at about $p = 0.3$. Further increments of $p$ increase the low temperature magnetization gradually. There is a large range of values of the $T = 0$ magnetization that can be achieved by tuning the Mn and the hole concentrations. This can be understood qualitatively in the following way: larger hole concentrations $px$ lead to larger Fermi wavevectors $k_F$. As a result, the oscillation between ferromagnetic and antiferromagnetic interactions described by the RKKY interaction appears at a shorter distance. If this distance becomes comparable to the average inter-spin distance, significant frustration is present in the system leading to suppressed low-T magnetization. When $p = 0.3$, the antiferromagnetic part seems to be dominant. The magnetization actually decreases as temperature is lowered below $0.4 J_{ef}$. This effect arises due to antiferromagnetic coupling between clusters as a result of the long-range nature of the RKKY interaction.

We have also investigated RKKY models with exchange anisotropy as discussed before. In all cases, the additional suppression of the low-T magnetization induced by the anisotropy is very small (less than 10%).
V. DISCUSSION

The major result that can be deduced from our simulation is that while exchange anisotropy can change the temperature scale at which ferromagnetism occurs in a model, it does not change the essential qualitative features such as the shape of the magnetization curve, or the form of the linear or susceptibility greatly above $T_c$, unless the ratio between the parallel and perpendicular exchanges is extremely different from 1. Below $T_c$, the anisotropy preserves a finite magnetization and linear susceptibility at $T = 0$. This effect is suppressed by higher connectivity (large $n_0$). [Locally the random lattice with $n_0 = 12$ is more symmetric than for $n_0 = 6$, so that the anisotropy a spin feels from one neighbor is more likely to be cancelled by the effects of other neighbors.] However, in general the effect of anisotropy is relatively weak, as it does not lower magnetization at $T = 0$ by more than 20%. The presence of antiferromagnetic interactions, as occur in oscillatory exchange interactions, such as in the RKKY model, appears to be much more important for lowering the magnetization at low temperature. Thus the large reduction in the magnetization seen in Ref. 1 can probably be attributed to RKKY interactions, rather than the effects of anisotropy in the exchanges.

Our result on the effects of moderately anisotropic exchange interactions on the magnetic properties of DMS are in substantial contrast with the results of Zarand and Janko. They found large differences between the low temperature magnetization (but similar Curie temperatures) in the isotropic and anisotropic cases. We are puzzled by this difference, but suggest that it may be due to the fact that they used an exponential cut-off in their exchange interaction. This cut-off may have damped the effect of anti-ferromagnetic interactions in the isotropic case, but since the parallel and perpendicular exchanges had different spatial dependences in their study, they may not have reduced the effect of anti-ferromagnetic exchanges in the anisotropic case.

There are a number of other interesting observations. The two types of anisotropy, corresponding to the cases $\lambda < 1$ and $\lambda > 1$ are qualitatively different. For $\lambda < 1$, the spins preferentially align along the line joining them, whilst for $\lambda > 1$ there is a preferred plane in which the spins may lie. This difference in dimensionality appears to explain why the magnetization is not suppressed as much at low temperatures for $\lambda > 1$ as compared to $\lambda < 1$, since it is easier for spins to relax from frustration in two rather than one dimensions.

Whilst anisotropic exchange interactions are one possibility which can lead to a reduction in the saturation magnetization at low temperatures, there are a number of other possibilities. Firstly, there are believed to be anti-ferromagnetic nearest neighbor interactions between Mn spins, that should have little effect due to the diluteness of the Mn spins, but could lead to a decrease in the saturation magnetization. Next is a theoretical proposal that there is an instability purely in the presence of disorder towards a non-collinear ground state. Another is the experimental observation that there are significant numbers of interstitial Mn that appear to be involved in compensation processes and thus do not polarize. It is not completely clear to what extent the saturation at low temperatures in Ga$_{1-x}$Mn$_x$As is due to non-participation of Mn spins due to the presence of Mn interstitial defects. However, given the recent progress in this area, it will probably not be long before an accurate estimate of the proportion of Mn that are participating in the ferromagnetism is known. When this is quantified, it should be possible to determine whether anisotropy need be included in realistic models of DMS and if so, how much. The carrier-mediated nature of the ferromagnetism also suggests that anisotropy may be important for transport, especially in the insulating phase, since hopping between sites will be preferred when the Mn spins have similar orientations.

We mention in passing that while anisotropy has small effect on the magnetization, it seems to have significant effect on the non-linear susceptibility at low temperature. This suggests that experimental investigations of the non-linear susceptibility might shed light on the magnetic state in DMS. It was recently suggested that for $x < 0.01$ and $x > 0.1$ in Ga$_{1-x}$Mn$_x$As, there may be a spin glass phase. Here we suggest that if there are strongly anisotropic exchange interactions, signatures might be seen in co-existence with ferromagnetism. If such spin-glass signatures are not seen in (Ga,Mn)As, they may be present in other insulating materials with lower carrier concentrations such as Ge:Mn.

In conclusion, there are still a number of outstanding questions as to the nature of the ferromagnetic state in DMS, and whether anisotropy plays an important role in these materials. This work should be of help in clarifying which types of models are likely to be affected by anisotropy and what types of experimental probes might help to detect it.

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To be more precise, each spin is coupled to at least two other neighboring spins. If a spin has less than 2 neighbors within a distance $R_c$, then we assume it to be coupled to its two closest neighbors (irrespective of how far they are). This avoids the existence of completely isolated spins in our model. For the values of $R_c$ we investigate, we find that only about 1-2% of spins are in this situation.