Monte Carlo study of the spin-glass phase of the site-diluted dipolar Ising model

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By tempered Monte Carlo simulations, we study site-diluted Ising systems of magnetic dipoles. All dipoles are randomly placed on a fraction \( x \) of all \( L^3 \) sites of a simple cubic lattice, and point along a given crystalline axis. For \( x_c < x \leq 1 \), where \( x_c \approx 0.65 \), we find an antiferromagnetic phase below a temperature which vanishes as \( x \to x_c \) from above. At lower values of \( x \), we find an equilibrium spin-glass (SG) phase below a temperature given by \( k_BT_{sg} \approx x \epsilon_d \), where \( \epsilon_d \) is a nearest neighbor dipole-dipole interaction energy. We study (a) the relative mean square deviation \( \Delta_q^2 \) of \( q \), where \( q \) is the SG overlap parameter, and (b) \( \xi_L/L \), where \( \xi_L \) is a correlation length. From their variation with temperature and system size, we determine \( T_{sg} \). In the SG phase, we find (i) the mean values \( \langle|q|\rangle \) and \( \langle q^2 \rangle \) decrease algebraically with \( L \) as \( L \) increases, (ii) double peaked, but wide, distributions of \( q/\langle|q|\rangle \) appear to be independent of \( L \), and (iii) \( \xi_L/L \) rises with \( L \) at constant \( T \), but extrapolations to \( 1/L \to 0 \) give finite values. All of this is consistent with quasi-long-range order in the SG phase.

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I. INTRODUCTION

The collective behavior of spin systems in which magnetic dipole-dipole interactions dominate has become the subject of considerable attention. These systems are rare in nature, although some ferroelectrics\textsuperscript{2} and magnetic crystals such as \( \text{LiHoF}_4 \), an insulating magnetic salt, have been known for decades to be well described by models of magnetic dipoles.\textsuperscript{2,4} Much of the renewed interest in systems of interacting dipoles comes from the experimental realization of magnetic nanoparticle\textsuperscript{5} arrays\textsuperscript{6,7} and of crystals of organometallic molecules.\textsuperscript{8} In these systems, particles up to some thousand Bohr magnetons behave as single spins. When closely packed in crystalline arrangements, dipolar interactions between them may induce magnetic order.\textsuperscript{9}

Anisotropy also plays an important role in ordering dipolar systems. The barrier energies \( E_a \) that must be overcome by spins in order to reverse their direction are often somewhat larger than the relevant dipolar energies \( E_d \). Then, collective effects can be observed when thermal energies are not sufficiently large to completely freeze spins directions. Their main effect is then to force spins to point up or down along the easy magnetization axis.\textsuperscript{2,4} Crystalline Ising dipolar systems (IDSs) are then reasonable models.\textsuperscript{2} These systems are clearly frustrated, since two different dipoles give rise to magnetic fields at any given site that are not in general collinear. Not surprisingly, IDSs are very sensitive to their spatial arrangement. Early work by Luttinger and Tisza established which type of magnetic order arises at low temperature for IDSs in each of the cubic lattices.\textsuperscript{11,12} More recently, we have obtained similar results by much simpler methods.\textsuperscript{12} For instance, BCC and \( \text{LiHoF}_4 \) like crystals are ferromagnetic ordered, but antiferromagnetic (AF) order obtains on simple cubic (SC) lattices. Competition between different interactions brings about a more exotic magnetic order, known as “spin ice”\textsuperscript{13} in diamond crystals.

Whether disorder in IDSs, together with the geometric frustration that comes with the dipolar interactions give rise to a thermodynamic spin-glass (SG) phase, is an interesting question.\textsuperscript{14} Many experiments\textsuperscript{15} as well as numerical simulations\textsuperscript{16} have shown that assemblies of classical magnetic moments placed at random, such as in frozen ferrofluids and diluted ferroelectric materials, exhibit the time dependent behavior, such as non-exponential relaxation and aging\textsuperscript{17} that is expected from SGs. However, search for evidence of an equilibrium SG phase has been hampered by the extremely slow relaxation that is inherent to these systems. In recent papers, we have given numerical evidence that supports the existence of an equilibrium SG phase in IDSs with randomly oriented axes both in fully occupied and in partially occupied SC lattices.\textsuperscript{18}

Site dilution is a rather simple way to introduce disorder in experimental realizations of IDS. Some early attempts to find a SG phase in \( \text{Eu}_x\text{Sr}_{1-x} \) \( \text{F}_4 \) led to negative results.\textsuperscript{20} By far the most scrutinized system for the last two decades has been \( \text{LiHo}_x\text{Y}_{1-x} \text{F}_4 \). In it, magnetic \( \text{Ho}^{3+} \) ions are substituted, with little distortion, by non magnetic \( \text{Y}^{3+} \) ions.\textsuperscript{21} A strong uniaxial anisotropy forces all spins to point up or down along the same axis at low temperatures. This parallel-axis-dipolar (PAD) system orders ferromagnetically a low temperature phase above \( x_c \approx 0.25 \). Below \( x_c \), transitions from a paramagnetic to a SG phase have been reported\textsuperscript{22–24}, but the opposite conclusion, that no such transition takes place, has been reached in Ref.\textsuperscript{24}. The issue is further obscured by quantum effects that may take place at \( x < 1 \).\textsuperscript{25}

Theoretical results suggest that diluted PAD models undergo a SG transition at low concentrations. An earlier study of bond-diluted Ising systems with long-range
interactions (including the dipolar case) found that SG order may exist at low temperatures in the limit of weak concentration.\textsuperscript{26} Mean field calculations for site-diluted PAD systems in FCC and BCC lattices predicted a SG phase for concentrations $0 < x < x_c$, where $x_c$ is the value above which ferromagnetic order ensues.\textsuperscript{27} More recently, Edwards-Anderson\textsuperscript{28} type models with power-law decaying interactions $J_{ij} \sim 1/r_{ij}^{\nu}$ have been studied.\textsuperscript{29,30} A 1D Ising Spin Glass model has been found to have a nonzero temperature SG phase transition for $\sigma < 1$.\textsuperscript{30} A 3D Ising systems with RKKY interactions (that decay with $1/r_{ij}^3$) have been predicted to lie in the same universality class as the 3D Ising Edwards-Anderson (EA) model with short range interactions.\textsuperscript{29}

Numerical methods have provided conflicting answers to the question of the existence of a SG phase in site diluted PAD models. Biltmo and Henelius\textsuperscript{31} have calculated that the ferromagnetic phase of LiHo$_x$Y$_{1-x}$F$_4$ extends down to $x_c \approx 0.24$, but found no SG phase at low temperatures for $x < x_c$.\textsuperscript{31} This is in contradiction with another MC simulation for the same system that finds a SG transition for concentrations $x = 0.065$ and 0.125.\textsuperscript{32} Numerical work has also been done on a PAD model on a SC lattice, using a Wang-landau MC method.\textsuperscript{33} No transition was found for $x < 0.2$.

Here we also simulate a PAD model on a SC lattice. Our justification for working with a SC lattice is as follows. Whereas such systems order AF in fully occupied SC lattices,\textsuperscript{11,12} instead of ferromagnetically, as in the LiHoY$_4$ lattice, the physics of PAD systems is not expected to depend on lattice structure for $x \ll 1$. A continuum should then lead to the same behavior. Furthermore, rescaling distance $r$ as $r \to r/\rho^{1/3}$, where $\rho$ is the spatial density of spins, is no different from redefining dipolar energies by $\varepsilon_d \to \rho \varepsilon_d$, since dipolar interactions decay as $r^{-3}$. Now, consider $k_B T_{sg}/n_d \varepsilon_d$ for any lattice structure, where $k_B$ is Boltzmann’s constant, $T_{sg}$ is the SG transition temperature, $n_d$ is the number of magnetic dipoles within a $d^3$ volume, and $\varepsilon_d$ is the smallest possible dipolar energy two parallel dipoles that are a distance $d$ apart can have. Clearly, $k_B T_{sg}/n_d \varepsilon_d$ must be independent of lattice structure for $x \ll 1$. This enables us to compare results for SC and LiHoF$_4$ lattices, or any other lattice, for $x \ll 1$. Such a comparison is made in Table I.

The main aim of this paper is to find, by means of MC simulations, whether an equilibrium SG phase exists in site diluted systems of dipoles, which are placed at random on the sites of a SC lattice and point up or down along a chosen principal axis. Since in the limit of low concentrations details of the lattice are expected to become irrelevant, our results have direct connection with the experimental and numerical work mentioned above. In this regard, we follow along the lines of Ref.\textsuperscript{32} But we aim to go further. It is our purpose to also find whether the SG phase of the PAD model behaves marginally, that is, it has quasi-long-range order (as the XY model\textsuperscript{25} in 2D), or whether it has spatially-extended states\textsuperscript{36} as in the droplet\textsuperscript{37} and replica-symmetry-breaking\textsuperscript{38} pictures of the SG phase.

![Table I: Spin-glass transition temperature for PAD systems. NIL is entered where a transition has been concluded not to take place. For LiHo$_x$Y$_{1-x}$F$_4$, we let $d = 5.175 \text{ Å}$, hence the mean number of spins in volume $d^3$ is $n_d = 1.926x$ (since unit cells of LiHoYF$_4$ are $5.175 \times 5.175 \times 10.75 \text{ Å}^3$ large and have 4 Ho ions each); furthermore, $x_c = 0.214 K$. On simple cubic lattices, we let $d = a$, hence $n_d = x$. $\chi_3$ is the nonlinear susceptibility, and $\nu$ is the critical exponent for the correlation length.](image)

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agreement with our MC results for $\xi_L/L$. All of this is consistent with quasi-long-range order in the SG phase. In Sec. IV C we find the best pair of values for $T_{sg}$ and $\nu$, to have curves $\xi_L/L$ for various values of $L$ collapse onto a single curve if plotted vs $(T/T_{sg} - 1)^{1/\nu}$ over the $T > T_{sg}$ range. The values given in Table I are obtained.

II. MODEL, METHOD, AND MEASURED QUANTITIES

A. Model

We consider site-diluted systems of Ising magnetic dipoles on a SC lattice. All dipoles point along the z axis of the lattice. Each site is occupied with probability $x$. The Hamiltonian is given by,

$$\mathcal{H} = \frac{1}{2} \sum_{ij} T_{ij} \sigma_i \sigma_j$$

where the sum is over all occupied sites $i$ and $j$ except $i = j$, $\sigma_i = \pm 1$ on any occupied site $i$,

$$T_{ij} = \varepsilon_a (a/r_{ij})^3 (1 - 3z_{ij}^2/r_{ij}^2),$$

$r_{ij}$ is the distance between $i$ and $j$ sites, $z_{ij}$ is the z component of $r_{ij}$, $\varepsilon_a$ is an energy, and $a$ is the SC lattice constant. In the following we give all temperatures and energies in terms of $\varepsilon_a/k_B$ and $\varepsilon_a$, respectively. Hence, $k_B T/n_a \varepsilon_a = T/x$ from here on.

This model is clearly an Ising model with long-range interactions where bond strengths $T_{ij}$ are determined by the dipole-dipole terms. Note that $T_{ij}$ signs are not distributed at random, but depend only on the orientation of vectors $r_{ij}$ on a SC lattice. This is to be contrasted with a random-axes dipolar model, (RAD) in which Ising dipoles point along directions $\mathbf{n}_i = (n_{i}^{\alpha}, \alpha = 1, 2, 3)$ that are chosen at random by sorting two independent random numbers for each site, introducing randomness on bond strengths $T_{ij}^{\alpha\beta}$. This is why PADs exhibit AF order at high concentration in contrast with RADs, that do not.

B. Method

We use periodic boundary conditions (PBC). As is usual for PBC, think of a periodic arrangement of replica that span all space beyond the system of interest. These replicas are exact copies of the Hamiltonian and of the spin configuration of the system of interest. Details of the PBC scheme we use can be found in Ref. 12. We let a spin on site $i$ interact through dipolar fields with all spins within an $L \times L \times L$ cube centered on it. No interactions with other spins are taken into account. This introduces an error which we show in Appendix I to vanish as $L \rightarrow \infty$, regardless of whether the system is in the paramagnetic, AF or SG phase. There is, therefore, no effect on the thermodynamic limit of the system of interest here. (The result we obtain in Appendix I is not applicable to an inhomogeneous ferromagnetic- phase or critical region- that may obtain on other lattices.)

In order to bypass energy barriers that can trap a system’s state at low temperatures in the glassy phase

| $x$ | 0.20 | $\Delta T$ | 0.02 | $T_0$ | 0.8 |
|-----|-----|---------|-----|-----|-----|
| $L$ | 4   | 6       | 8   | 10  |     |
| $T_n$ | 0.06 | 0.06   | 0.06 | 0.12 |     |
| $N_r$ | 8500 | 3800   | 1000 | 800  |     |
| $t_0$ | $5 \times 10^7$ | $5 \times 10^7$ | $5 \times 10^7$ | $5 \times 10^7$ |     |
| $x$ | 0.35 | $\Delta T$ | 0.05 | $T_0$ | 2.0 |
| $L$ | 4   | 6       | 8   | 10  | 12  |
| $T_n$ | 0.05 | 0.05   | 0.05 | 0.275 | 0.35 |
| $N_r$ | 9000 | 5000   | 1100 | 380  | 200 |
| $t_0$ | $4 \times 10^6$ | $4 \times 10^6$ | $4 \times 10^6$ | $4 \times 10^6$ |     |
| $x$ | 0.50 | $\Delta T$ | 0.05 | $T_0$ | 2.0 |
| $L$ | 4   | 6       | 8   | 10  |     |
| $T_n$ | 0.10 | 0.10   | 0.20 | 0.30 |     |
| $N_r$ | 1400 | 500    | 800  | 300  |     |
| $t_0$ | $5 \times 10^7$ | $5 \times 10^7$ | $4 \times 10^7$ |     |
| $x$ | 0.60 | $\Delta T$ | 0.1 | $T_0$ | 2.0 |
| $L$ | 4   | 6       | 8   | 10  |     |
| $T_n$ | 0.1  | 0.10   | 0.10 | 0.30 |     |
| $N_r$ | 1400 | 900    | 1400 | 540  |     |
| $t_0$ | $4 \times 10^6$ | $4 \times 10^6$ | $4 \times 10^6$ | $4 \times 10^6$ |     |
| $x$ | 0.65 | $\Delta T$ | 0.1 | $T_0$ | 3.0 |
| $L$ | 4   | 6       | 8   | 10  |     |
| $T_n$ | 0.1  | 0.10   | 0.10 | 0.30 |     |
| $N_r$ | 1400 | 900    | 1400 | 540  |     |
| $t_0$ | $4 \times 10^6$ | $4 \times 10^6$ | $4 \times 10^6$ | $4 \times 10^6$ |     |
| $x$ | 0.70 | $\Delta T$ | 0.1 | $T_0$ | 3.0 |
| $L$ | 4   | 6       | 8   | 10  |     |
| $T_n$ | 0.1  | 0.10   | 0.10 | 0.30 |     |
| $N_r$ | 1400 | 900    | 1400 | 540  |     |
| $t_0$ | $4 \times 10^6$ | $4 \times 10^6$ | $4 \times 10^6$ | $4 \times 10^6$ |     |
| $x$ | 0.75 | $\Delta T$ | 0.1 | $T_0$ | 3.0 |
| $L$ | 4   | 6       | 8   | 10  |     |
| $T_n$ | 0.1  | 0.10   | 0.10 | 0.10 |     |
| $N_r$ | 1000 | 200    | 100  | 100  |     |
| $t_0$ | $4 \times 10^6$ | $4 \times 10^6$ | $2 \times 10^6$ | $2 \times 10^6$ |     |
| $x$ | 0.80 | $\Delta T$ | 0.1 | $T_0$ | 3.0 |
| $L$ | 4   | 6       | 8   | 10  |     |
| $T_n$ | 0.1  | 0.10   | 0.10 | 0.10 |     |
| $N_r$ | 600  | 200    | 220  | 100  |     |
| $t_0$ | $4 \times 10^6$ | $4 \times 10^6$ | $10^6$ | $10^6$ |     |
we have used the parallel tempered Monte Carlo (TMC) algorithm.\cite{39,43} We apply the TMC algorithm as follows. We run in parallel a set of $n$ identical systems at equally spaced temperatures $T_i$, given by $T_i = T_0 - i \Delta T$ where $i = 0, \cdots, n - 1$ and $\Delta T > 0$. By identical we mean here that all $n$ systems have the same quenched distribution of empty sites, though each system starts from an independently chosen initial condition. We apply the TMC algorithm to any given system in two steps. In the first step, system $i$ evolves independently for $8$ MC sweeps under the standard single-spin-flip Metropolis algorithm\cite{33} (Owing to dipolar interactions, the MC sweep time scales as $N^2$, where $N$ is the number of spins.) We calculate the probability distribution $P_i$ of empty sites, though each system starts from an independently chosen initial condition. We apply the TMC algorithm as follows. In the second step, we give system $i$ a chance to exchange states with system $i + 1$ evolving at a lower temperature $T_i - \Delta T$. We accept exchanges with probability $P = 1$ if $\delta E = E_i - E_{i+1} < 0$, and $P = \exp(-\Delta \beta \delta E)$ otherwise, where $\Delta \beta = 1/T_{i+1} - 1/T_i$. The cycle is complete when $i$ has been swept from 0 to $n - 2$. Thus, we associate eight MC sweeps with each cycle. For the simulation to converge at low temperatures it is important to choose $\Delta T$ small enough to allow frequent state exchanges between systems. This will often be fulfilled if $\Delta \beta \Delta T \lesssim 1$. The required condition, $\Delta T \lesssim T/\sqrt{Nc}$, follows for $\Delta T$ where $c$ is the specific heat per spin. Then, we obtain appropriate values for $\Delta T$ from inspection of plots of the specific heat vs $T$\cite{18}. We find it helpful to have the highest temperature $T_0$ at least twice as large as what we expect to be the transition temperature between the paramagnetic and the ordered phase for obtaining equilibrium results in the ordered phase.

In our simulations the $n$ identical systems start from completely disordered spin configurations. We need equilibration times $t_0$ of at least $4 \times 10^6$ MC sweeps for $x \leq 0.7$ for systems with a number dipoles $N \geq 200$ (see at the end of this section for details on how we choose $t_0$). Thermal averages come from averaging over the time range $[t_0, 2t_0]$. We further average over $N_r$ samples with different realizations of disorder. Values of the parameters for all TMC runs are given in Table I.

C. Measured quantities

We next specify the quantities we calculate. We obtain the specific heat from the temperature derivative of the energy. For the staggered magnetization, we define, as befits a PAD model on a SC lattice,\cite{12}

$$m = N^{-1} \sum_i \sigma_i (-1)^{x(i)+y(i)}$$

where $x(i)$ and $y(i)$ are the space coordinates of site $i$. We calculate the probability distribution $P_m$, as well as the moments

$$m_n = \langle |m|^n \rangle,$$

for $n = 1, 2$, where $\langle \rangle$ stand for averages over time and over a number $N_r$ of system samples with different quenched disorder. Unless otherwise stated, time averages are performed over a time range $t_0 < t < 2t_0$, and $t_0$ is chosen as specified below in order to ensure equilibrium. We make use of these moments to calculate the staggered susceptibility and the mean square deviation of $|m|/m_1$, that is,

$$\Delta^2 = \frac{m_2}{m_1^2} - 1.$$  \hspace{1cm} (5)

In order to spot SG behavior, we also calculate the Edwards-Anderson overlap parameter,\cite{28}

$$q = N^{-1} \sum_j \phi_j$$  \hspace{1cm} (6)

where

$$\phi_j = \sigma_j^{(1)} \sigma_j^{(2)}$$  \hspace{1cm} (7)

$\sigma^{(1)}_j$ and $\sigma^{(2)}_j$ are the spins on site $j$ of identical replicas (1) and (2) of the system of interest. As usual, identical replicas have the same Hamiltonian, and are at the same temperature, but are in uncorrelated states. Clearly, $q$ is a measure of the spin configuration overlap between the two replicas. As we do for $m$, we calculate the probability distribution $P_q$ as well as the moments $q_1 = \langle |q| \rangle$ and $q_2 = \langle q^2 \rangle$, in analogy to Eq. (5). The SG susceptibility $\chi_q$ is given by $Nq^2$. Finally, we also make use of the relative mean square deviation of $q$, $\Delta^2_q = q_2/q_1 - 1$.

We need to make sure that equilibrium is reached before we start taking measurements. To this end, we define a time dependent spin overlap $\tilde{q}$, not between pairs of identical systems, but between spin configurations of the same system at two different times $t_0$ and $t_1 = t_0 + t$ of the same TMC run,

$$\tilde{q}(t_0, t) = N^{-1} \sum_j \sigma_j(t_0)\sigma_j(t_0 + t).$$

Let $\tilde{q}_2(t_0, t) = \langle |\tilde{q}(t_0, t)|^2 \rangle$. Suppose thermal equilibrium is reached long before time $t_0$ has elapsed. Then, $\tilde{q}_2(t_0, t) \rightarrow q_2$ at some time $t$ long before $t = t_0$. Plots of $q_2(t_0, t)$ vs $t$, for $10^{-6}t_0 < t < t_0$, for $t_0 = 10^7$ MC sweeps, are shown in Fig. 1 for $x = 0.20$ and various values of $T$. Plots of $q_2$, obtained by averaging $q^2$ over time, not starting at $t = t_0$, as we do everywhere else in order to obtain equilibrium values, but starting at $t = 0$, from an initial random spin configuration, are also shown in Fig. 1 for comparison. Note that both quantities do become approximately equal when $t \gtrsim 10^5$ MC sweeps. In order to obtain equilibrium results, we have always chosen sufficiently large values of $t_0$ to make sure that
TABLE II. The AF phase is defined by the staggered magnetization \( m \), which is given by:

\[ m^2 = \frac{4}{N} \sum_{i,j} | \langle \phi_i | \phi_j \rangle |^2 \] 

where \( \langle \phi_i | \phi_j \rangle \) is the overlap of the |\( \xi \rangle \) states. The AF phase is characterized by the presence of long-range order, which can be detected using various probes, such as the specific heat or the staggered magnetization.

In summary, the AF phase is characterized by the presence of long-range order and the emergence of a macroscopic correlation length \( \xi_\infty \). The transition to the AF phase is driven by changes in the system's parameters, leading to the formation of an ordering transition, as shown in the inset of Fig. 2b. The phase boundary between the paramagnetic and AF phases is determined by the competition between the random interactions and the cooperative effects that lead to order.

We return to this point in the discussion of Eq. (11).

Plots of the specific heat \( C \) vs \( T \) are shown in the insets of Figs. 3a and 3b. Note the sharp variation of \( C \) near the transition temperature, indicating the presence of a phase transition.
FIG. 3: (Color online) (a) Staggered magnetization $m_1$ vs $T$ for $x = 0.8$. Icons ◊, □, ●, and △ stand for $L = 10, 8, 6$ and $4$ respectively. Lines are only guides to the eye. Note $m_1$ grows with $L$ at low temperature, consistently with an AF phase. In the inset, specific heat vs. $T$ for the same values of $x$ and of system sizes. The sharp variation $C$ with respect to $T$ near $T = 1.5$ is consistent with an AF phase transition thereon. (b) Same as in (a) but for $x = 0.6$. Note (i) $m_1$ decreases with $L$ at all temperatures, consistently with the nonexistence of an AF phase, and (ii) a rounded specific heat, consistent with a SG transition. In all panels, error bars are shown only where they are larger than symbol sizes.

FIG. 4: (Color online) (a) Log-log plots of $m_2$ versus $N$ for $x = 0.7$ and the values of $T$ shown. Continuous lines are guides to the eye, except for the straight line over the data points for $T = 1.2$, which is for $1/N^{0.35}$. A dashed line shows the slope one expects for a macroscopic paramagnet. (b) Same as in (a) but for $x = 0.5$. In all panels, error bars are smaller than symbol sizes.

$C$ vs $T$ near $T = 1.5$, in Fig. 4a, as one expects from a paramagnetic-AF phase transition. Note also how, as one expects for a paramagnetic-SG transition, $C$ varies smoothly for a smaller value of $x$, in Fig. 3b).

For further information about the extent of the AF phase, we now examine how $m$ varies with $N$ for some values of $x$ and of $T$. Compare the log-log plots of $m_2$ versus the number of dipoles $N$ on Figs. 4a and 4b, respectively. The data points in Fig. 4a are consistent with a second order phase transition from a magnetically disordered phase, above $T = 1.2(1)$, for which $Nm_2 = O(1)$, to a strong long-range order below $T = 1.2(1)$, where $m_2 = O(1)$. Note that $m_2 \sim 1/N^p$ at $T = 1.2$. From the definition of $\eta$ (see Sec. 11 or Ref. 46), $3p = 1 + \eta$ follows, which gives $\eta = 0.05$. We are however not too interested here in such details of the critical behavior on the $T = T_{AF}(x)$ line. In Fig. 4b, $m_2$ vs $N$ plots show faster than algebraic decay with $N$. This shows we are then beyond the bounds of the AF phase. We have followed this criterion as a first approach in establishing the boundary of the AF phase. Plots of $m_1$ (instead of $m_2$) vs $N$ show the same qualitative behavior.

We draw more quantitative results about the AF phase

FIG. 5: (Color online) (a) Plots of $\Delta g_x^2$ vs $T$, for $x = 0.7$. ◆, ◊, ○, and × are for $L = 10, 8, 6$ and $4$, respectively. Lines are guides to the eye. The thick dashed-line is for the macroscopic paramagnetic limit $\pi/2 - 1$. (b) Same as in (a) but for $x = 0.6$. (c) Plots of $\Delta q_m^2$ vs $T$, for $x = 0.7$. Symbols are as in (a). (d) Same as in (c) but for $x = 0.6$. Error bars are shown only where they are larger than symbol sizes.

FIG. 6: (Color online) Semilog plots of $q_x^2$ versus $T$ for $x = 0.2$, and $L = 10$, ◆, $L = 8$ (□), $L = 6$ (○), and $L = 4$ (●). All error bars are smaller than symbol sizes.
boundary from the behavior of the relative uncertainty $\Delta^2_m$. We first outline how we expect $\Delta^2_m$ to behave as a function of $T$ and $x$ in the various magnetic phases. It clearly follows from its definition in Eq. (4) that $\Delta^2_m \to 0$ as $N \to \infty$ in the AF phase. It also follows immediately from the the law of large numbers that, in the paramagnetic phase, $\Delta^2_m \to \pi/2 - 1$ as $N \to \infty$. These two statements imply that curves of $\Delta^2_m$ vs $T$ for various values of $N$ cross at the phase boundary between the paramagnetic and AF phases. We make use of this fact to quantitatively determine the AF-paramagnet phase boundary. The same criterion can be applied to the AF-SG phase boundary. To see why this is so, note that, the plots in Fig. 6 imply that curves of $\Delta^2_m$ vs $T$ are shown in Figs. 5a and 5b for $x = 0.7$ and 0.6, respectively. The signature of an AF phase below $T \approx 1.2$ clearly shows up in Fig. 6a. We have thus established all points of the AF phase boundary shown in Fig. 2 for $x \geq 0.7$. For the low temperature portion of the phase boundary (near $x = 0.65$) this procedure is not very effective. From Fig. 6a, we infer that the AF boundary line must drop to a $T = 0$ value at some $x > 0.60$. The three data points shown for $x \approx 0.65$ and $T < 1$ are obtained from plots such as the one shown in the inset of Fig. 2 for $T = 0.4$.

IV. THE SG PHASE

In this section, we report numerical results we draw from tempered MC calculations for $q_2$, for distributions of $q$, and for $\xi_L$. Because we expect, from the argument given in Sec. I, lattice independent behavior for $x \ll 1$, we emphasize the results we have obtained for the two smallest values of $x$ we have dealt with, $x = 0.2$ and $x = 0.35$ (that is, $x \approx 0.30x_0$ and $x \approx 0.50x_0$).

A plot of $q_2$ versus $T$ is shown in Fig. 6. Note that $q_2$ decreases as $N$ increases, even at low temperatures. We have found similar behavior for other values of $x$ satisfying $x \lesssim x_0$. Inspection of this figure raises the question of whether $q_2$ vanishes as $L \to \infty$. In order to advance in this direction, we do log-log plots of $q_2$ vs $N$, which we show in Figs. 6a, 6b, and 6c, for the values of $x$ shown therein. The data points in these three figures seem consistent with, $q_2 \sim N^{-p}$ for $T/x \lesssim 1$, where $3p = 1 + \eta$, as follows from the definition of $\eta$ in Sec. V.B (see also Ref. 46). $\chi^2$ values for $q_2 \sim N^{-p}$ fits to sets of data points, for $T/x \lesssim 1$ (for which they are appropriate) as well as for $T/x \gtrsim 1$ (for which they are not appropriate), are given in Table III. Plots of $q_1$ vs $N$ show the same qualitative behavior. All of this is in accordance with quasi-long-range order. We return to this point below and in Sec. V.B.

Reading off values of $p$ from plots shown in Figs. 6a, 6b, and 6c, we obtain $\eta$ for $x \leq 0.5$ and various values of $T$. The relation $\eta = -1 + a_x(T/x)^2$ fits the data rather well for all $T/x \lesssim 1$, if we let $a_x = 0.76$, 0.98, 1.18 for $x = 0.2$, 0.35, 0.5, respectively. In order to be able to conclude that $q(T_{sg})$ varies with $x$, we would need to know $T_{sg}$ within an error of 10%. Unfortunately, we find below (in Sec. V.A) an error in $T_{sg}$ which is not much smaller than 10%.

For higher values of $T/x$, $q_2$ vs $N$ curves downwards, as expected for the paramagnetic phase. Approximate values of $T_{sg}$ can thus be obtained from such plots, but more accurate methods are given below. It is reassuring to see in Figs. 6b, 6c, and 6d, the values of $q_2$ we have obtained agree, within errors, with the values for $q_2$.

We next give distributions of $q$ we have found. We make use of a normalized distribution $P_q(q_x)$, where...
TABLE III: $\chi^2$ values for two-parameter $q_2 = c/N^p$ fits to sets of data points for $q_2$ vs $T$ displayed in Figs. 1a-c. As usual, we define $\chi^2 = \chi^2/df$, where $df$ is the number of data points in each set minus the number of fitting parameters (2, here). The largest errors $\Delta q_2$ of $q_2$ from all data points for each $x$ and $T$ are also given.

| $x$ | $\chi^2$ | $\Delta q_2$ | $T$ | $\chi^2$ | $\Delta q_2$ | $T$ | $\chi^2$ | $\Delta q_2$ |
|-----|-----------|--------------|-----|-----------|--------------|-----|-----------|--------------|
| 0.50 | 1.29      | 0.01         | 0.20 | 0.84      | 0.01         | 0.30 | 0.91      | 0.01         |
|      | 0.21      | 0.01         | 0.70 | 0.30      | 0.01         | 0.35 | 0.38      | 0.01         |
|      | 0.02       | 0.16        | 0.52 | 0.02      | 0.18         | 0.01 | 0.01      | 0.01         |
|      | 0.16       | 0.03        | 0.45 | 0.20      | 0.12         | 0.50 | 0.01      | 0.01         |
|      | 1.70       | 0.008       | 0.50 | 0.004     | 0.22         | 0.60 | 0.004     | 0.20         |
|      | 15.09      | 0.003       | 0.60 | 0.003     | 1.24         | 0.80 | 0.003     | 0.38         |

$q_r = q/q_1$. In macroscopic paramagnets, $q_r$ is expected to be normally distributed, as follows from the law of large numbers and the fact that spin-spin correlations lengths are then finite. On the other hand, $P_q = [\delta(q_r - 1) + \delta(q_r - 1)]/2$, where $\delta$ is the Dirac delta function, in a SG phase, according to the droplet picture of SGs. Plots of $P_q$ vs $q$ are shown for $x = 0.2$ in Figs. 8a, 8b, and 8c. Clearly, $P_q(q_r)$ drifts with system size in Fig. 8c, for $T = 0.28$. Our results are consistent with $P_q(q_r) \to (1/\pi) \exp(-q_r^2/\pi)$ as $N \to \infty$, which is in accordance with a paramagnetic phase. On the other hand, we find for lower temperatures double peak distributions in Figs. 8a and Fig. 8c that are fairly broad and, within errors, do not change with $N$. This is contrary to the prediction of the droplet-model theory of SGs. From these graphs we conclude that $0.16 < T_{sg} < 0.26$ for $x = 0.2$. Analogous plots for $x = 0.35$ (not shown) give $0.30 < T_{sg} < 0.45$.

Results for the scale free quantity $\Delta^2_q$ follow. Recall that, as explained for $\Delta^2_m$, $\Delta^2_q \to \pi/2 - 1$ as $N \to \infty$ in the paramagnetic phase, vanishes when there is strong long-range order, and goes, at the critical temperature, to some intermediate value that is size independent. This is as shown in Fig. 5a for $x = 0.7$ where curves for various values of $N$ cross at $T_{AF}$. Figures 5b and 5c look rather similar, because $q$ and $m$ are not qualitatively different in the AF phase. This is not so for $x < x_c$, where there is no AF order. Figures 5b and 5c for $x = 0.6$ show that, within errors, curves of $\Delta^2_q$ vs $T$ for different system sizes merge (not cross) near $T = 0.65$, while $\Delta^2_q$ increases with $N$ for all temperatures. Similarly, $\Delta^2_q$ vs $T$ curves merge, for $x = 0.65$, near $T = 0.75$ (not shown). Plots of $\Delta^2_q$ vs $T/x$ are shown in Figs. 9a, 9b, and 9c for lower concentrations.

We notice that curves in Figs. 9a, 9b, and 9c differ only slightly. This follows from the argument given in Sec. I, which shows that all physical quantities for three dimensional dipolar systems can only be functions of $T/x$ for $x \ll 1$. The data points in Fig. 9a show that $\Delta^2_q \to \pi/2 - 1$ as $N \to \infty$, for $T/x \gtrsim 1$, as expected for the paramagnetic phase.

Curves for $\Delta^2_q$ vs $T$ seem to merge at a lower temperature, near $T/x = 0.9$. However, closer scrutiny shows that these curves actually cross, albeit at very small glancing angles. This can be appreciated in Figs. 9a, 9b, and 9c, where plots of the ratios $\Delta^2_q(L)/\Delta^2_q(4)$ vs. $T$ are given for various values of $L$, for $x = 0.5$, $x = 0.35$, and $x = 0.2$, respectively. Note that the weak dependence of $\Delta^2_q$ with system size at low temperatures is in accordance with our result that $P_q(q_r)$ does not change appreciably with system size below $T_{sg}$. This point is further elaborated in Sec. V B.

Following the lead of Refs. 48 and 51, who have found that $4\xi_{L}/L$ (defined in Sec. II C) crosses at $T_{sg}$ and spreads out as $T$ decreases below $T_{sg}$ for the EA model in 3D, we next examine how $4\xi_{L}/L$ behaves for the PAD model. As pointed out in Sec. I and Table I, this has already been done for the PAD model on a LiH$_2$O$_{1-x}$Y$_4$ lattice by Kam and Gingras. As we also point out in Sec. I, we aim to explore the behavior of the PAD model, not only near $T_{sg}$, but also deep into the SG
phase. Recall that $\xi_L$ becomes a true correlation length when $\xi_L/L \ll 1$. Then, in the paramagnetic phase, $\xi_L/L \sim O(1/L)$, therefore decreasing as $L$ increases. At $T = T_{sg}$, $\xi_L/L$ must become size independent, as expected for a scale free quantity. The inferences one can make about the nature of the condensed phase from the behavior of $\xi_L$ where $T < T_{sg}$ is the subject of Sec. V B.

Without further comment, we next report our results. Plots of $\xi_L/L$ versus $T/x$ are shown in Figs. 10a and 10b for $x = 0.35$ and 0.2, respectively. Note that curves spread out above and below $T/x \sim 1$. For $x = 0.35$, curves for all $L$ cross at $T_{sg}/x = 0.95(5)$. On the other hand, the temperatures where pairs of curves for lengths $L_2$ and $L_1$ cross for $x = 0.2$ decrease as lengths $L_2$ and $L_1$ increase (see Fig. 10b), pointing to a $T_{sg}/x \lesssim 1.1$.

V. EXISTENCE AND NATURE OF THE SG PHASE

In this section we examine the numerical results given in the previous section. We (i) arrive at values for $T_{sg}$ as a function of $x$, (ii) show that weak long-range order is consistent with our results for the SG phase, and (iii) draw values for the critical exponent $\nu$ for various values of $x$. 
A. The value of $T_{sg}$

Recall first that $\Delta_q^2$ vs $T$ curves for different values of $L$ are supposed to come together as $T$ approaches $T_{sg}$ from above. This behavior is exhibited in Figs. 9a-c. A closer view of how such curves actually meet at $T = T_{sg}$ is offered in Figs. 10d-f, where plots of $y(L, 4)$ versus $T/x$, where $y(L, L') = \Delta_q^2(L)/\Delta_q^2(L')$, are shown. One aims to find the $L \to \infty$ and $L' \to \infty$ limit of $y(L, L') = 1$, which gives the value of $T_{sg}$. We find that $y(L, L') = 1$ at values of $T/x$ that increase with $L$ and $L'$, which is reassuring, because it shows that $T_{sg}$ does not vanish. Furthermore, we draw the following lower bounds from the plots in Figs. 10d-f, $T_{sg}/x \gtrsim 0.95$, $0.8$, $0.95$, for $x = 0.5$, $0.35$, $0.20$, respectively.

We obtain a complementary determination of $T_{sg}$ from the intersection of $\xi_L/L$ vs $T$ curves. This is as is sometimes done for the EA$^{20-22}$ and PAD$^{22}$ models. We obtain, from Fig. 11a, $T_{sg}/x \approx 0.95$ for $x = 0.35$. In Fig. 11b, we see that $\xi_L/L$ vs $T$ curves meet at decreasingly smaller values of $T$ as $L$ increases. We thus obtain $T_{sg}/x \lesssim 1.1$ for $x = 0.2$.

From these two complementary determinations, we arrive at: $T_{sg}/x = 1.0(1)$ for $x \lesssim 0.5$.

An aside follows about the result by Snider and Yu$^{23}$ that $T_{sg} = 0$ for $x = 0.045, 0.12$ or $0.2$. This is, of course, in clear contradiction with our results. Their conclusions come from their work with the Wang-Landau$^{24}$ variation of the MC algorithm. Their evidence is from plots of $T_g$ versus $N$, where $T_g$ is the temperature at which $P_g$ becomes flat at. This procedure makes sense because $T_g \to T_{sg}$ as $N \to \infty$. They found $T_g$ to vanish as $N^{-1/2}$ for several $x$ values, including $x = 0.2$. We now repeat this procedure using our own data, including the ones for $x = 0.2$. In Fig. 11b, we plot the flattest distributions we found for $x = 0.2$ and $L = 4$, 8, and 10. Note in passing that all scaled distributions coincide and have therefore the same value of $\Delta_q^2$. Plots of the values of $T_g/x$ we have obtained for $x = 0.5, 0.35$, and $0.2$ are shown in Fig. 11b. Our data points are in clear contrast to the $T_g \sim N^{-1/2}$ trend of Ref. 33, and point to $T_{sg}/x \approx 1$. Whether this disagreement comes from using a different Monte Carlo method, or from the unusual definition of $q$ in Ref. 33 we do not know.

B. Marginal behavior

Here we discuss how various pieces of evidence (including crossings of $\xi_L/L$ vs $T$ curves) lead us to the conclusion that the SG phase of the PAD model behaves marginally. That is to say, that $\langle q^2 \rangle \to 0$ and $\chi_{sg} \to \infty$ in the macroscopic limit.

The variation of $\langle q^2 \rangle$ with $L$ for various temperatures, exhibited in Figs. 4d-e, has already been considered in Sec. IV. For all $x < x_c$, $T < T_{sg}$, and all system sizes we have studied, we find no deviation from $\langle q^2 \rangle \sim L^{-\langle 1+\eta \rangle}$. Nor do we find any size dependence in $P_q(q_n)$. This is illustrated in Figs. 5 and c, and is in accordance with the behavior of the distribution of the magnetization that is observed$^{10}$ in the condensed phase of the 2D XY model. Note that the variation of $\Delta_q^2$ with system size is a measure of the variation of $P_q(q_{n1})$. The very small changes we have observed in $\Delta_q^2$ as $L$ varies in the PAD model for all $T \lesssim T_{sg}$ turn out to be smaller than the corresponding changes in the XY model$^{10}$ This is, of course, in marked contrast with the behavior one expects of the corresponding quantity for a strongly ordered system, such as the droplet model of SGs or an ordinary ferromagnet, in which $\Delta_q^2 \to 0$ in the macroscopic limit of the ordered phase. Neither do our results fit into a RSB scenario$^{10}$ in which $q_2$ does not vanish as $L \to \infty$ and would have $P_q(q_{n1})$ changing with system size, since $P_q(q_{n1})$ is wide and does not change with system size in the SG phase.

We now analyze the data we have for $\xi_L$. First, we outline how we expect $\xi_L/L$ to spread out as $T$ decreases below $T_{sg}$ in various SG scenarios.

(i) Condensate with short range order fluctuations. In such a SG phase, $q_2 \neq 0$ and $\langle \phi_0 \phi_1 \rangle - \langle \phi_0 \rangle \langle \phi_1 \rangle$ would be short ranged. This would fit into the droplet model of

![FIG. 12: (Color online) (a) Semilog plots of $\xi_L/L$ versus 1/L for x = 0.35, and T/x = 0.143 ($\bullet$), T/x = 0.286 (■), T/x = 0.571 ($\bigstar$), T/x = 0.857 ($\blacktriangle$), T/x = 1.00 ($\blacktriangleleft$), T/x = 1.14 ($\bigcirc$), $T/x = 1.43$ (□), $T/x = 1.71$ (○), and $T/x = 2.00$ ($\blacklozenge$). (b) Same as in (a), but for for x = 0.20, and T/x = 0.300 ($\bullet$), T/x = 0.500 (■), T/x = 0.700 ($\bigstar$), T/x = 1.00 ($\blacktriangle$), T/x = 1.10 ($\blacktriangleleft$), T/x = 1.30 ($\bigcirc$), T/x = 1.50 (□), T/x = 2.00 (○), and $T/x = 2.50$ ($\blacklozenge$). All errors are: between 2% and 3% in (a), and between 2% and 4% in (b), and are thus hidden behind the icons. In both (a) and (b), the straight-dashed lines give $\chi_n^2 < 1$ fitting values, except for $T/x = 1.0$ in (b), for which $\chi_n^2 = 3.3$.](http://example.com/Figure12.png)
spin glasses. It then follows straightforwardly from its definition [Eq. (9)] that \( \xi^2_L/L^2 \sim L^d \). Here, \( d = 3 \), and there is nothing in the plots of \( \xi_L/L \) vs \( 1/L \), which are shown in Figs. 12a and 12b, to suggest that \( \xi^2_L/L^2 \sim L^d \) at any nonzero temperature.

(ii) \textbf{Condensate with long range order fluctuations.}

Let \( \langle A \rangle_q \) be the thermal average of \( A \) over all states with a given \( q \) value. Clearly, \( \langle A \rangle = \int \langle A \rangle_q P_q dq \). Assume \( q_2 \neq 0 \), and \( \int [\langle \phi_0 \phi_r \rangle_q - \langle \phi \rangle_q^2] P_q dq = G(r) \), where,

\[
G(r) = \frac{A}{\nu^{d-2+\eta}},
\]

for \( r \gg a \), where \( A \) is a constant. This behavior fits in with the RSB picture. Then, it follows from its definition [Eq. (9)] that \( \xi^2_L/L^2 \sim L^{1+\eta} \). Recall, from Sec. IV that \( \eta \approx -1 + (T/T_{sg})^2 \) in the SG phase. Evidence for \( \xi^2_L/L^2 \sim L^{1+\eta} \) appears neither in Fig. 12a nor in Fig. 12b.

(iii) \textbf{Marginal behavior.}

Then, \( q_2 = 0 \) and \( \langle \phi_0 \phi_r \rangle = G(r) \). This is as in the KT theory of the 2D XY model. It then follows straightforwardly from the definition of \( \xi_L/L \) that \( \xi_L/L \) becomes independent of \( L \) for very large \( L \). This is precisely the outcome from \( 1/L \to 0 \) extrapolations of the straight lines shown in Fig. 12a and 12b for all \( T/x \lesssim 1 \).

Note also in Figs. 12a and 12b that curves for \( \xi_L/L \) vs \( 1/L \) become steeper as \( T \) decreases below \( T/x \approx 1 \). Now, recall from above that \( q_2 \neq 0 \) implies \( \xi^2_L/L^2 \sim L^d \) and \( \xi^2_L/L^2 \sim L^{1+\eta} \), for short- and long-range fluctuations from the condensate. Note further that \( |1+\eta| \) decreases as \( T \) decreases. This would lead to \( \xi_L/L \) vs \( 1/L \) curves which do not become steeper as \( T \) decreases below \( T/x \approx 1 \), which is in clear contradiction with the observed behavior. This is an additional piece of evidence for quasi-long-range order.

Thus, the most straightforward interpretation of the data shown in Figs. 12a and 12b leads us to suspect that the SG phase in the PAD model behaves marginally. This might seem to be in contradiction to the fact that \( \xi_L/L \) curves do cross, as shown in Fig. 10 and that, as pointed out in Ref. 41, \( \xi_L/L \) vs \( T \) curves merge, not cross, for the 2D XY model, as \( T \to T_{sg} \) from above. (Indeed, no crossings occur for even much smaller 2D XY systems than the ones for which data points are shown in Ref. 41.) We next give a specific example in order to illustrate how both merging and spreading out as \( T \) decreases below \( T_{sg} \) can take place, depending on the some details in \( G(r) \).

We first calculate \( \xi_L/L \) from \( \langle \phi_0 \phi_r \rangle = G(r) \) and Eq. (12) for all \( r \) except that \( G(r) = 1 \) for all \( r \leq 1 \). To proceed, we let \( A \approx 0.67 \) for \( T \leq T_{sg} \) but not too close to \( T = 0 \), where one expects \( A = 1 \). We are not interested here in the \( T > T_{sg} \) range, but we nevertheless then let \( A \to A e^{-r/\xi_{sc}} \), \( \xi_{sc} = 7(T/T_{sg} - 1)^{-\nu} \), and \( \nu = 1 \), which is roughly the value we obtain below (see Sect. V C). We make use of \( \eta = -1 + (T/T_{sg})^2 \), which we have found in Sec. IV. Finally, in order to be able to make comparisons with our MC results, which we have obtained for periodic
boundary conditions, we let in Eq. (12),

$$r \rightarrow Q^{-1} \left[ \sum_{\alpha=1}^{3} \sin^2(Qr_{\alpha}) \right]^{1/2},$$

(13)

where $Q = \pi / L$ and $r = (r_1, r_2, r_3)$. Straightforward numerical implementation of Eq. (12) yields the data points that are plotted in Fig. 10. Note the resemblance between Fig. 10 and Figs. 10 and 10, which follow from our MC calculations.

Merging of $\xi_L / L$ curves at $T = T_{sg}$ as $T$ decreases is obtained for all $L \geq 4$ if, instead of $A = 0.667$, we let $3A = 3 - (T/T_{sg})^2$. Note that $A(T_{sg}) = 0.667$ and $A(0) = 1$. If, on the other hand, one lets $3A = 3 - (T/T_{sg})^s$ and $0 < s \lesssim 0.2$, which satisfies the same end point conditions, one obtains plots for $\xi_L / L$ vs $T$ which look much like the ones shown in Figs. 10.

To summarize, all our data (including spreading out of $\xi_L / L$ curves as $T$ decreases below $T_{sg}$) are consistent with marginal behavior in which the correlation length diverges at $T_{sg}$ as in a conventional phase transition, but weak-long-range order occurs below $T_{sg}$, as in the 2D XY model.

C. The $\nu$ exponent

In accordance with the ones above, we look for the values of $\nu$ and $T_{sg}$ which best collapse $\xi_L / L$ vs $(T/T_{sg} - 1)L^{1/\nu}$ plots for various values of $L$ into a single curve for temperatures above $T_{sg}$. The best results, exhibited in Figs. 10 and 10, for $x = 0.35$ and $x = 0.20$, are obtained with $T_{sg}/x = 1.0(1)$ and $\nu = 0.95$. Note the data points scatter below $T_{sg}$. This is as expected, and is consistent with quasi-long range order in the SG phase, since $\xi_L / L$ becomes independent of $L$ and $\nu$ for sufficiently large $L$. Note that, as in the EA model, $L = 4$ seems to be too small to scale properly.

VI. DISCUSSION

By tempered Monte Carlo calculations, we have studied an Ising model on a simple cubic lattice. There are only dipole-dipole interactions. Spins (randomly) occupy only a fraction $x$ of all lattice sites. We have calculated the entire phase diagram of the system. It is shown in Fig. 2. We have also provided strong evidence for the existence of a SG phase for $0 < x < x_c$, where $x_c = 0.65(5)$. The SG transition temperature is given by $T_{sg}(x) \simeq x$. We have argued in Sec. I that this result carries over into other lattices if (i) $x \ll 1$, and (ii) we replace the latter expression for $T_{sg}$ by $k_B T_{sg} = n_d \xi_d$ (see Table I). How have we arrived at this conclusion is described in Sec. IV-A.

We have not dwelt on the applicability of our MC results to experiments. That is beyond the scope of this paper. We nevertheless make a few comments. Recall first that, as we argue in Sec. I, lattice structure is of no consequence for very dilute PAD models. Then, $T_{sg}$ as well as the temperature $T_m$ where the specific heat takes its maximum value can only depend (as in the MC simulations of Ref. 31) on $n_d \xi_d$ (see Table I). We notice in Table I values for $T_{sg}$ do not fully comply with this rule. In addition, in very dilute LiHo$_2$Y$_{1-x}$F$_4$ systems, $T_m$ hardly changes with $x$. There are several sources for the discrepancies between experiments on very dilute LiHo$_2$Y$_{1-x}$F$_4$ and the PAD model. Quantum effects seem to play a role in experiments on very dilute LiHo$_2$Y$_{1-x}$F$_4$ systems. This is not so surprising, since tunneling can become relevant when barrier energies become overwhelmingly large. However, we do not expect small perturbations that bring about tunneling and concomitant time dependent effects to have a significant effect on equilibrium properties, which is the subject of this paper. In addition, exchange couplings among nearest neighbor spins 31,48 are disregarded in the PAD model we study. Note, however, that the effect of nearest neighbor interactions must vanish as $x \rightarrow 0$. Clustering of the spatial distribution of dipoles can also lead to discrepancies.32 None of the above can however account for (i) the numerical differences between the MC results (see Table I ) of Tam and Gingras 32 and ours, nor can they account for the more serious discrepancy with (ii) Ref. 33, which we discuss in some detail in Sec. VI-A. Numerical (not too large) discrepancies notwithstanding, our results support the ones from Tam and Gingras 32 that the dilute PAD model does have a SG phase. On the other hand, for the roots of the discrepancies with experimental results (see Table I ) on dilute LiHo$_2$Y$_{1-x}$F$_4$ systems, we have no clear picture.

As for the nature of the SG phase, all of our results are consistent with quasi-long-range order. Full details are given in Sec. VI-B. We know of no previous study of the nature of the SG phase of the PAD model with which to compare our results. (Only the critical behavior of a PAD model is examined in Ref. 32.) On the other hand, our conclusion for the PAD model can be compared with and one drawn for the EA model in Refs. 40-42. They are both based on the behavior of $\xi_L / L$ vs $T$ curves for various values of $L$. The conclusions differ, not so much because of the data, but because we have looked at the data differently (see Sec. VI-B and Refs. 40-42).

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Appendix A: WHY WE DO NOT DO EWALD SUMS

We consider site-diluted systems of Ising magnetic dipoles in a cubic box of $L^3$ sites on a SC lattice. All dipoles point along the $z$ axis of the lattice. Each site is occupied with probability $x$. We assume thermal equilibrium. We show two things in this appendix. We first show that the contribution $\Delta h$ to the magnetic field $h$ at the center of such box, coming from a periodic arrangement of replicas that span all space beyond the system of interest (the “outer space”) within an arbitrarily large cube which is centered on the system of interest, vanishes as $L \to \infty$ if the system is not in a ferromagnetic phase or close to its Curie temperature. More specifically, we show that if $\langle s\rangle < 0$ is short ranged, and the system is homogeneous (including antiferromagnetically ordered states), then

$$\langle \Delta h^2 \rangle \to 0$$  \hspace{1cm} (A1)

as $L \to \infty$, where $\langle \ldots \rangle$ stands for an average over both a canonical ensemble and (site occupation) disorder. Note that we are not imposing the condition that $\langle s\rangle < 0$ is short ranged, and recall (1) that in general $\sum_j \langle s_i s_j \rangle - \langle s_i \rangle < 0$ vanishes as $L \to \infty$ if the system is not in a ferromagnetic phase or close to its Curie temperature. More specifically, we show that if $\langle s\rangle < 0$ is short ranged, and the system is homogeneous (including antiferromagnetically ordered states), then

$$\langle \Delta h^2 \rangle \to 0$$  \hspace{1cm} (A1)

as $L \to \infty$, where $\langle \ldots \rangle$ stands for an average over both a canonical ensemble and (site occupation) disorder. Note that we are not imposing the condition that $\langle s\rangle < 0$ is short ranged, and recall (1) that in general $\sum_j \langle s_i s_j \rangle - \langle s_i \rangle = T \chi_m$, where $\chi_m$ is the magnetic susceptibility per site, and (2) that $T \chi_m \lesssim 1$ for spin glasses. Equation (A1) clearly indicates that thermodynamic limits can be obtained from Monte Carlo calculations for systems of various sizes in which contributions from the outer space are disregarded. Finally, explicit numerical evidence, Fig. 14, to this effect is also given.

To begin, let $h = \sum_j T_{ij} s_j$ (where $\sum_j T_{ij} s_j$ be the sum is over all occupied sites within (outside) a cubic box of $L \times L \times L$ sites, centered on $i$. Therefore,

$$\Delta h^2 = \sum_{n,m} T_{in}T_{im} s_n s_m$$  \hspace{1cm} (A2)

where the double sum is over all occupied sites in the outer space. Let

$$f(r_n) = \sum_j \frac{\varepsilon a^3}{|r_n + R_j|^3} \left[ 1 - \frac{3(z_n + z_j)^2}{|r_n + R_j|^2} \right],$$  \hspace{1cm} (A3)

where $R_j$ is the position of the outer $j$th box, $r_n$ is the $n$-th site’s position with respect to the center of the box, and the sum is over all outer boxes. Equation (A2) then becomes,

$$\Delta h^2 = \sum_{n,m} f(r_n) f(r_m) s_n s_m$$  \hspace{1cm} (A4)

where the sum is over all occupied sites within our system of interest. We now replace $s_n$ by $\langle s_n \rangle + \delta s_n$, and similarly for $s_m$, in the equation above. Now, it can be checked straightforwardly (i) that $\sum_m f(r_m) \langle s_n \rangle = 0$ if $\langle s_n \rangle$ is either independent of $n$ (which would not hold for a ferromagnet with domains) and (ii) that $\sum_m f(r_m) \langle s_n \rangle \to 0$ as $L \to \infty$ if $\langle s_n \rangle$ follows an antiferromagnetic order (which, for up and down spins with dipolar interactions on a SC lattice, is a checkerboard-like arrangement of up and down ferromagnetic columns). Performing thermal and disorder averages over the above equation, one then obtains,

$$\langle \Delta h^2 \rangle \to \sum_{n,m} f(r_n) f(r_m) \langle \delta s_n \delta s_m \rangle.$$  \hspace{1cm} (A5)

as $L \to \infty$. Now, $f(r)$ varies smoothly within the system, whence

$$\langle \Delta h^2 \rangle \to \sum_n \sum_m |f(r_n)|^2 \langle \delta s_n \delta s_m \rangle$$  \hspace{1cm} (A6)

if $\langle \delta s_n \delta s_m \rangle \simeq 0$ unless $|r_n - r_m| \ll L$. Finally, $\sum_n |f(r_n)|^2 = \frac{b \langle s_n^2 \rangle}{L^3}$, where $b \simeq 7.6$ if $L \gg 1$, as follows straightforwardly by numerical integration. Replacement of $\sum_m \langle \delta s_n \delta s_m \rangle$ by $T \chi_m$ gives Eq. (A1) if $T \chi_m$ is finite. For all the parameters used in our MC calculations, we have found that $T \chi_m \lesssim 1$.

The difference $\Delta \xi_L / L$ between the correlation lengths we report and the ones obtained when Ewald sums are included for $x = 0.35$, is $\bullet$ $L = 4$ and $\circ$ $L = 8$. These data points follow from averages over $10^4$ and $10^3$ systems samples, for $L = 4$ and $L = 6$, respectively. The same sample realizations were used for the calculations with and without Ewald sums.
\[ L = 6. \] The results are clearly consistent with a \( \Delta \xi_L/L \) that vanishes in the thermodynamic limit.
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