Nature of the spin-glass phase in dense packings of Ising dipoles with random anisotropy axes

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Abstract
Using tempered Monte Carlo simulations, we study the spin-glass phase of dense packings of Ising dipoles pointing along random axes. We consider systems of dipoles (i) placed on the sites of a simple cubic lattice with lattice constant \(d\), and (ii) placed at the center of random close packed spheres of diameter \(d\) that occupy 64\% of the volume. For both cases, we find a spin-glass phase below a certain temperature \(T_{sg}\). By analysing the data obtained for the overlap parameter, the associated correlation length, as well as the statistics of the overlap distributions of individual samples, we find a behavior consistent with quasi-long-range order in the spin-glass phase, similar to the one previously found in strongly diluted dipolar systems.

Keywords: classical spin models, spin glasses and other random magnets, frustrated magnetism, ensembles of nanoparticles

(Some figures may appear in colour only in the online journal)

1. Introduction
Disorder and frustration are determinants for the onset of spin-glass (SG) phases. The Edwards–Anderson (EA) model \([1, 2]\) is the simplest model presenting SG and including both ingredients \([3]\). Interactions in the EA model are short ranged and have random signs.

Systems characterized by long range interactions and strong dilution can also include disorder and frustration. In dipolar crystals where the dipoles occupy at random a small fraction of the available sites of the crystalline lattice, this randomness, together with the anisotropy of the dipolar interaction, creates a network of arbitrarily distributed ferromagnetic and antiferromagnetic couplings. For example, SG behavior has been detected in diluted samples of LiHoF\(_4\) which can be described as systems of Ising dipoles (DIS) \([4]\). This one and other similar diluted crystals are often called ‘atomic spin-glasses’.

Advances in nanoscience \([5]\) have brought a new type of dipolar SG made of dense ensembles of identical interacting nanoparticles (NPs) \([6, 7]\) that behave as single dipoles. NP exhibit effective anisotropies that oblige the dipoles to lie along easy axes, and force them to overcome a certain energy barrier \(E_a\) during spin flips. For high enough \(E_a\), nanoparticles behave like Ising dipoles. When, in order to disregard exchange interactions, NP are either coated or plunged in an insulating medium or just neatly separated, the dipolar becomes the only relevant particle–particle interaction. Such disordered arrays of NP have been obtained from colloidal dispersions of particles in frozen fluids \([8]\), or by compacting powders of coated NP in granular solids \([7, 9]\).

It is at high enough densities, when the dipolar interparticle energies \(E_{dd}\) become comparable to the anisotropy energies \(E_a\), that a cooperative behavior among dipoles arises at low temperatures \([7, 10]\). Then, frozen disorder in the position of each NP and/or in its random orientation together with frustration (that comes from dipolar interactions) result in SG behavior \([11]\). These types of SG, made of nanoparticles instead of magnetic atoms, are called ‘super SG’. Very recently, SG behavior clearly governed by dipolar interactions.
has been observed in random close packed (RCP) samples [12], where the typical volume fraction can be as large as 64%.

In the present paper, we investigate by Monte Carlo (MC) simulations whether the SG character of these dense systems and of diluted atomic spin-glasses may differ or not. Numerical simulations of disordered systems of dipoles have shown non-equilibrium signatures of SG at low temperature [13–15] and, irrespective of the relative dipolar interaction strength, an Ising-like behavior of the dipoles [14]. An MC work for a fully occupied simple cubic (SC) lattice of Ising dipoles with randomly oriented axes [16] found an equilibrium SG transition, but no clear-cut results about the nature of the low temperature phase were obtained. For strongly diluted DIS [17–19] the MC simulations also exhibit an equilibrium SG phase below a temperature $T_{SG}$, but data are consistent with quasi-long-range [20] order (like in the 2D XY model) in the SG phase [18, 19].

Neither the droplet model [21] nor a mean-field description [22] of SG fit in with such marginal behavior. The mean-field Parisi’s solution for SG is represented by the so-called replica symmetry breaking scenario (RSB) [22]. The low temperature phase depicted by this scenario possesses many quasi-degenerated states separated by infinite barriers. A paradigmatic model that exhibits RSB is the Sherrington–Kirkpatrick (SK) model [23, 24], where the couplings between pairs of spins are chosen randomly to be ferromagnetic or antiferromagnetic regardless of the spin–spin distance. However, the applicability of an RSB scenario to more realistic (i.e. non mean-field) SG models is still controversial [3, 25].

To grasp to what extent the degree of dilution may play a role in the onset of a dipolar SG phase, consider an ensemble of dipoles randomly distributed in a certain volume. If they are strongly diluted, the probability of having two such dipoles a distance $r$ apart is $\rho(r)dr \propto 4\pi r^2 dr$. Since dipole interactions $J$ are proportional to $1/r^3$, the distribution of couplings must follow the functional law $P(J)dJ \propto dJ/J^2$. Contrarily, if the dipoles are densely packed, possible overlaps among nearest particles invalidate the trend $\rho(r) \propto r^2$, and consequently also the distribution $P(J) \propto 1/J^2$ [26]. Therefore, it makes sense to entertain the possibility that the physics of dense packings of dipoles may be different from that of the strongly diluted ones. We shall make these differences in $\rho(r)$ and $P(J)$ more quantitative in section 2.1.

The purpose of the present work is to investigate by tempered MC simulations the SG phase of dense packings of randomly oriented Ising dipoles and check whether or not there are qualitative differences in the marginal behavior observed for very diluted systems.

Concretely, we consider arrays of dipoles placed on the sites of a fully-occupied simple cubic (SC) lattice, and ensembles of dipoles placed at the center of RCP spheres that occupy a 64% fraction of the entire volume. This is the maximum allowed fraction for compactly packed, arbitrarily placed spheres [27]. We investigate the low temperature phases of the system by measuring the overlap parameter $q$ between equilibrium configurations, its associated correlation length, as well as sample-to-sample fluctuations of probability distributions of $q$ for different realizations of disorder.

The paper is organized as follows. In section 2 we define in detail the model and the types of dense packings, explain the MC algorithm and define the quantities we measure. The results are presented in section 3 with some concluding remarks in section 4.

2. Models, method and measured quantities

2.1 Models

We study the low temperature behavior of dense packings of $N$ identical magnetic NP that behave as single magnetic dipoles. The NP are labelled with $i = 1, \ldots, N$. Each one is a hard sphere of diameter $d$ carrying a permanent pointlike magnetic moment $\vec{m}_i = \mu \sigma_i \hat{\mu}_i$ at its center. $\hat{\mu}_i$ is the local easy-axis and $\sigma_i = \pm 1$ is a sign representing the moment $\vec{m}_i$ pointing up or down along $\hat{\mu}_i$. $\mu \equiv ||\vec{m}_i||$ is equal for all dipoles. Mimicking real dense packings of NP, $\hat{\mu}_i$ axes will be left frozen along random directions. Magnetic moments are coupled solely by dipolar interactions. The Hamiltonian can be expressed in the manifestly Ising-like form

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j,$$

where

$$J_{ij} = \varepsilon_d \left( \frac{d}{r_{ij}} \right)^3 \left( \vec{a}_i \cdot \vec{a}_j - \frac{3(\vec{a}_i \cdot \vec{r}_{ij})(\vec{a}_j \cdot \vec{r}_{ij})}{r_{ij}^2} \right).$$

$\varepsilon_d = \mu_0 \mu^2/(4\pi d^3)$ is an energy and $\mu_0$ the magnetic permeability in vacuum. $\vec{r}_{ij}$ is the vector position of dipole $j$ viewed from dipole $i$. Clearly $r_{ij} \equiv ||\vec{r}_{ij}||$. The summation runs over all pairs of particles $i$ and $j$, except $i = j$. The arbitrariness of directions $\vec{a}_i$ makes the distribution of $J_{ij}$ signs to appear random-like.

In our simulations, we flip dipoles up and down along their easy axes. Given that we are not interested in time dependent properties controlled by the interplay between local anisotropy and interparticle dipolar energies, we do not try to replicate how dipoles overcome anisotropy barriers. Rather, we reproduce the collective evolution that follows when the system is allowed to explore the rough free-energy landscape inherent to SG and relax to equilibrium.

We shall analyse by MC simulations two different types of dense packings of identical spheres. In the first type the spheres are placed on the nodes of SC lattices with lattice spacing $d$ and in the second type the spheres are allocated in random close packings (RCP) with volume fraction $\phi = 0.64$. Note that, stemming from the spatial disorder in $\vec{r}_{ij}$, there is an additional source of randomness in RCP. Both types of packings are collectively called random axial dipole systems (RADS). We do not expect to see relevant differences in the behavior of the two packings because both are rather homogeneous and dominated by the random easy-axis distribution.

For comparison, we also study the SK model: a set of $N$ Ising spins $\sigma_i = \pm 1$ where every spin interacts with all the others. The interaction energies between the spins at sites
are chosen. Besides the disorder in the orientations of vectors \( \hat{a}_i \), RCP systems include another source of disorder, namely the positions of the centers of the spheres.

\[ J_{ij} \sigma_i \sigma_j \] with \( J_{ij} \sim r_{ij}^{-3} \), not only the geometry of the ensemble is affected, but also the distribution of couplings itself, \( P(J) \), as shown in figure 1(b). As is clear from equation (2), \( -2 \leq J/\varepsilon_d \leq +2 \).

For each one of the above-described models, we have employed \( N_s \) independent samples, where each sample \( J \) is a concrete realization of quenched disorder. For RAD systems this disorder means choosing the orientations of vectors \( \hat{a}_i \) randomly, while a sample for the SK model is defined by the distribution of signs in \( J_{ij} \). Besides the disorder in the orientations of \( \hat{a}_i \), RCP systems include another source of disorder, namely the positions of the centers of the spheres.

\[ L = 18.66d \] for 

\[ \phi = 0.01 \] \( J = (N\pi/60)^{1/3} \) for \( \phi = 0.64 \). The growth of \( \phi \) with \( N \) is why we have not made \( \varepsilon_d \) smaller with increasing \( N \). For RAD systems in SC lattices with \( N = 1000 \), we could only employ 1400 samples because of computer time limitations.

\[ T_{\text{min}} \] and \( T_{\text{max}} \) are the lowest (highest) temperature and \( \Delta \) is the temperature step in our TMC simulations. The number of simulation sweeps for equilibration is \( t_0 \). The number of samples with different realizations of quenched disorder is \( N_s \).

**Table 1.** Simulation parameters for SC and RCP systems. \( N \) is the number of dipoles, \( T_{\text{min}} \) (\( T_{\text{max}} \)) is the lowest (highest) temperature and \( \Delta \) is the temperature step in our TMC simulations. The number of simulation sweeps for equilibration is \( t_0 \). Measurements are taken in the time interval \([t_0, 2t_0] \). The number of samples with different realizations of quenched disorder is \( N_s \).

| \( N \) | \( T_{\text{min}} \) | \( T_{\text{max}} \) | \( \Delta \) | \( t_0 \) | \( N_s \) |
|-------|-----------------|-----------------|---------|--------|-------|
| 64    | 0.2             | 2.1             | 0.05    | 8 \times 10^4 | 5100 |
| 125   | 0.2             | 2.1             | 0.05    | 8 \times 10^6 | 10000 |
| 216   | 0.2             | 2.1             | 0.05    | 8 \times 10^6 | 8000 |
| 343   | 0.2             | 2.1             | 0.05    | 8 \times 10^6 | 4800 |
| 512   | 0.2             | 2.1             | 0.05    | 8 \times 10^6 | 5100 |
| 1000  | 0.6             | 2.1             | 0.05    | 10^7     | 1400 |

**Table 2.** Same as in table 1 for the SK model.

| \( N \) | \( T_{\text{min}} \) | \( T_{\text{max}} \) | \( \Delta \) | \( t_0 \) | \( N_s \) |
|-------|-----------------|-----------------|---------|--------|-------|
| 64    | 0.16            | 1.60            | 0.04    | 10^8   | 10^5  |
| 216   | 0.16            | 1.60            | 0.04    | 10^8   | 1.4 \times 10^5 |
| 512   | 0.16            | 1.60            | 0.04    | 2 \times 10^8 | 10^5 |

Once all these parameters have been fixed, the only freedoms left are the signs \( \sigma_i \). A concrete configuration during MC simulations is thus a given set of \( N \) signs \( \{ \sigma_i \} \).

To fix the positions in RCP systems, the Lubachevsky–Stillinger (LS) algorithm [29, 30] has been used. This algorithm starts by placing a Poisson distribution of \( N \) identical hard spheres in a cube whose edges have the length \( L = 1 \). At the beginning the spheres occupy a volume fraction \( \phi = 0.2 \). Then assuming periodic boundary conditions, we let the spheres move and collide according to Newton dynamics while growing in size until the sample eventually reaches the maximum volume fraction \( \phi = 0.64 \) [30]. The growth is performed at a sufficiently high rate to avoid the system ending up in a crystalline state. Proceeding in this way, the system eventually gets stuck in a disordered state [27, 30]. Once the LS algorithm has stopped, all dimensions are rescaled such that spheres reach a diameter \( d = 1 \) and the cube size \( L \) becomes \( L = (N\pi/60)^{1/3} \) for \( \phi = 0.64 \).

We shall identify the size of the system by the number \( N \) of spheres inside it. The number of samples \( N_s \) is listed in tables 1 and 2 for every size \( N \). Because of the inherent lack of self-averaging, measurements for systems in an SG phase present size independent statistical errors. This is why we have not made \( N_s \) smaller with increasing \( N \).
2.3. The simulation method

Periodic boundary conditions are also imposed during the simulations. We let each dipole \( i \) interact with the other dipoles within an \( L \times L \times L \) box centered on \( i \). This box includes dipoles from the repeated copies (by periodicity) of the cube. In order to take into account the slowly decaying long-range dipole–dipole interaction, we perform Ewalds’ summations [31] wherever necessary. Dipoles are screened by Gaussians with standard deviation \( \frac{1}{2} \alpha \) that allow us to split the computation of the dipolar energy into two rapidly convergent sums, one in real space and the other in reciprocal space. We evaluate the sum in real space using the normal image convention, with a cutoff \( r_c = L/2 \). A reciprocal space cutoff \( k_c \) is also introduced for the sum in the reciprocal space. We have chosen \( k_c = 10 \), and \( \alpha = 7.9/L \) as a good compromise between accuracy and computational speed [32]. Finally, given that our system is expected to exhibit zero magnetization, we have used a surrounding permeability \( \mu' = 1 \).

A parallel tempered Monte Carlo (TMС) algorithm is used for simulations [33]. It consists of running a set of \( n \) identical replicas of each sample \( \mathcal{J} \) in parallel at various temperatures in the interval \([T_{\min}, T_{\max}]\) with a separation \( \Delta \) between neighboring temperatures. Each replica starts from a completely disordered configuration. We apply the TMC algorithm in two steps. In the first one, the \( n \) replicas of the sample \( \mathcal{J} \) evolve independently for 8 MC sweeps [34]. All the replicas are evolved at temperatures in the interval \([0,2\Delta]\) with a spacing \( \Delta \) between the temperatures. During each step, the temperature \( T \) of replicas evolving at temperatures \( T \) and \( T + \Delta \) are chosen in such a way that detailed balance [33]. These exchanges allow all replicas to drift back and forth along the temperature axis, and choose \( \Delta \) such that at least 30% of all attempted exchanges are accepted.

Two types of averagings were considered: over thermalized states of a given sample \( \mathcal{J} \) and over the \( N_s \) samples. Depending on the information we were seeking, measurements were sometimes done after the first of the averages and sometimes after both. The first average is realized within the time interval \([t_0, 2t_0]\), where \( t_0 \) is the equilibration time (values of \( t_0 \) are shown in tables 1 and 2). Given an observable \( u \), \( u, \mathcal{J} \) stands for the thermal average of sample \( \mathcal{J} \) and \( \langle u \rangle \) for the average of the latter over samples. \( \langle u \rangle \) will often be denoted by merely the same symbol that denotes the observable itself, \( u \). The values of various parameters used in the simulation runs are given in tables 1 and 2.

2.4. Observables

The SG behavior has been investigated by studying the overlap parameter [1],

\[ q \equiv \frac{1}{N} \sum_j \sigma_j^{(1)} \sigma_j^{(2)}, \tag{3} \]

where, given a sample \( \mathcal{J} \), \( \sigma_j^{(1)} \) and \( \sigma_j^{(2)} \) are the signs at site \( j \) of two replicas, called (1) and (2), that evolve independently in time.

We then measure \( q_2 \equiv \langle q^2 \rangle \) and \( q_1 \equiv \langle |q| \rangle \) and, for each sample \( \mathcal{J} \) the overlap probability distribution \( p_{\mathcal{J}}(q) \), as well as its average over samples, that we denote simply as \( p(q) \). We also measure the mean square deviations of \( p_{\mathcal{J}}(q) \) from the average \( p(q) \) over samples,

\[ \Delta p(q)^2 \equiv \langle (p_{\mathcal{J}}(q) - p(q))^2 \rangle. \tag{4} \]

As usual in SG work [35, 36], the correlation length \( \xi_\perp \) is computed by

\[ \xi_\perp \equiv \frac{1}{4 \sin^2(k/2)} \left( \langle |q(k)|^2 \rangle - 1 \right), \tag{5} \]

where \( q(k) \) is

\[ q(k) \equiv \frac{1}{N} \sum_j \psi_j e^{i\vec{r}_j \cdot \vec{k}}, \tag{6} \]

with \( \psi_j \equiv \sigma_j^{(1)} \sigma_j^{(2)} \) at the position \( \vec{r}_j \) of dipole \( j \), \( \vec{k} = (2\pi/L, 0, 0) \) and \( k = ||\vec{k}|| = 2\pi/L \). Due to the isotropy of the RAD systems, all directions \( \vec{k} \) are equivalent.

In the paramagnetic phase, the correlation function \( \langle \psi_j \psi_j \rangle \) decays as \( \exp(-r/\xi_\perp) \) where \( r \equiv ||\vec{r}|| \) and \( \xi_\perp \) is the correlation length in the thermodynamic limit. \( \xi_\perp \) in equation (5) provides an approximation of \( \xi_\perp \). The closer \( \xi_\perp/L \) is to zero, the better that approximation is [36].

This is not the case for an ordered phase. Consider, for example, strong long–range order with short–range fluctuations. That is, \( \langle \psi_j \psi_j \rangle \) does not vanish as \( r \to \infty \) and \( \langle \psi_j \psi_j \rangle - \langle \psi_j \rangle \langle \psi_j \rangle \propto \exp(-r/\xi_\perp) \). In such a case, \( \xi_\perp \) in equation (5) diverges as \( L^{5/2} \) and is not related with \( \xi_\perp \) [36]. Following current usage, we shall nevertheless refer to \( \xi_\perp \) as ‘the correlation length’. Note that, in contrast to \( p(q) \) and its first moments, \( \xi_\perp \) includes spatial variations of the overlap \( q \).

2.5. Equilibration times

To make sure that thermal equilibrium is reached before we start taking measures, we followed the same procedure as in [19] by defining for two replicas of a single sample \( \mathcal{J} \) the overlap \( q_i \) at time \( t \) and the average \( q_2(t) \) of its square over all samples. Equilibrium is reached when \( q_2(t) \) attains a plateau. In order to confirm this result, a second overlap \( \tilde{q}_{0,\mathcal{J}} \)

\[ \tilde{q}_{0,\mathcal{J}} \equiv \frac{1}{N} \sum_j \sigma_j(t_0) \sigma_j(t_0 + t), \tag{7} \]

between configurations of a single replica taken at times \( t_0 \) and \( t_0 + t \) is measured as a function of \( t \). Equilibrium requires that the corresponding average \( \tilde{q}_2(t_0, t) \) remains stuck to the above plateau as \( t \) varies [19].

Plots of \( \tilde{q}_2(t_0, t) \) and \( q_2(t) \) versus \( t \) are shown in figures 2(a) and (b) for RAD systems on SC lattices (RCP) for \( t_0 = 4 \times 10^6 \) MC sweeps with \( N = 512 \) and \( T = 0.2 \), the lowest value of \( T \) in the series of TMC simulations.
Figure 2. (a) Semilog plots of $\bar{q}_2(t_0, t)$ (○) and $\tilde{q}_2(t)$ (●) versus time $t$ (measured in MC sweeps) for SC packings of 512 dipoles evolving at $T = 0.2$, the lowest temperature of our TMC simulations. Here, $t_0 = 4 \times 10^6$ MC sweeps. Data points at time $t$ stand for an average over the time interval $[t, 1.2t]$ and over $10^5$ samples. (b) The same for RCP.

Expectedly, equilibration takes longer for larger roughness in the free-energy landscape [37]. Numerous spikes in the overlap distributions $p_{\theta, \varphi}(q)$ are associated with samples having several pure states [38]. Moreover, the symmetry of the plots of overlap distributions like the ones shown in figure 6(a) for SC constitute an additional check that all the samples are well equilibrated.

3. Results

3.1. The SG phase

In this section we report and interpret the numerical results obtained for $q_2$ and $\xi_L/L$.

A log–log plot of $q_2$ versus $N$ at different values of $T$ is shown in figure 3 for RAD systems in SC lattices and RCP arrangements. For both models $q_2$ decreases as $N$ increases, and this occurs at all temperatures. For $T < 0.8$ and the system sizes studied, data in this figure are consistent with an algebraic decay $q_2 \sim N^{-(1+\eta)}$, following the usual definition of exponent $\eta$ [39]. Plots of $q_2$ versus $N$ (not shown) exhibit the same qualitative behavior. All of this is in accordance with quasi-long-range order. We will return to this point below. From the plots in figure 3, one could extract $\eta$ for various values of $T$. The relation $\eta = -1 + a T^2$ fits the data well with $a = 0.44(3)$ for both SC and RCP. Our results disagree with an RSB scenario, in which $q_2$ does not vanish as $N \rightarrow \infty$. For even higher temperatures than those shown in figure 3, $q_2$ versus $N$ curves bend downwards, as expected for the paramagnetic phase. Approximate values of $T_{sg}$ can thus be obtained from such plots, but we prefer to determine this temperature with the more accurate method given below (see figure 4).

We next examine the behavior of $\xi_L/L$ near $T_{sg}$ and also deep into the SG phase. Recall that $\xi_L/L$ falls off as $1/L$ in the paramagnetic phase, while it increases as $L$ increases in the ordered phase. At the temperature $T_{sg}$ where the system passes from one phase to the other, we can reasonably expect that curves of $\xi_L/L$ versus $T$ for different values of $N$ cross, enabling us to extract $T_{sg}$. At $T_{sg}$, $\xi_L/L$ becomes size independent, as expected for a scale free quantity.

Plots of $\xi_L/L$ versus $T$ are shown in figure 4 for different values of $N$ on SC (figure 4(a)) and RCP (figure 4(b)) arrays. All curves intersect at a precise temperature value and this fact allows us to determine $T_{sg}$ as is done for EA [35, 36] and dipolar SG [17, 18] models. For our SC (RCP) systems, curves cross at $T_{sg} = 0.57(2)$ ($T_{sg} = 0.78(3)$).

We now focus on the data for $\xi_L$ at low temperatures and check if they are consistent with the algebraic decay of $q_2$ exhibited in figure 3.

![Figure 2](image_url)

![Figure 3](image_url)

![Figure 4](image_url)
The value of $q_2$ is non zero in the SG phase of the droplet picture and fluctuations are short ranged [21]. It then follows that $\xi_4/L^2 \sim L^3$. In none of the temperatures do the plots of $\xi_4/L$ versus $1/L$, shown in figure 5, suggest that trend.

Let us imagine that the connected correlation function $G(r) = \langle \psi_1(0) \psi_2(r) \rangle - \langle \psi_1(0) \rangle \langle \psi_2(r) \rangle$ was to decay as $G(r) \sim 1/r^{(1+\eta)}$ for $r \to \infty$ while having $q_2 \neq 0$ like in the RSB picture. It then follows from equation (5) that $\xi_4^2/L^2 \sim L^{(1+\eta)}$ [18]. On the other hand, we deduced from figure 3 that $1 + \eta$ is an increasing function of $T$. All these properties entail that $\xi_4/L$ in figure 5 should decrease with $1/L$ at a slower pace at lower temperatures. However, figure 5 exhibits the opposite behavior: the downward trend at lower temperatures. However, figure 5 exhibits the opposite behavior: the downward trend at lower temperatures. Hence, we conclude from figure 5 that there is no evidence for the decay $G(r) \sim 1/r^{(1+\eta)}$ at large $r$ while having $q_2 \neq 0$.

Finally, let us consider $G(r) \sim 1/r^{(1+\eta)}$ and $q_2 = 0$ as in the 2D XY model [20]. It then follows that $\xi_4/L$ does not diverge as $L \to \infty$. This is the outcome from $1/L \to 0$ extrapolations of the dashed straight lines shown in figure 5 for $T < T_{sg}$. Thus, a straightforward interpretation of the data shown in figure 5 is that the SG phase for our densely packed RAD systems behaves marginally\(^4\).

3.2. Overlap distributions

It is interesting to study the SG behavior in individual samples. In figure 6(a) we plot $p_J(q)$ versus $q$ for three samples at temperature $T = 0.2$ for RADs on an SC lattice. $p_J(q)$ distributions are markedly sample-dependent and exhibit several sharp spikes centered well away from $q = \pm 1$. Similar behavior has been found for the EA and SK models [38, 40]. The positions and heights of the spikes in the region $q \in (-Q, Q)$ for, say, $Q = \frac{1}{2}$ change greatly from sample to sample. These inner peaks arise from overlaps between different pure states. We name these spikes cross-overlap (CO) spikes. Their number in $p_J(q)$ is closely related to the number of pure states $N$. At high temperatures (not shown), thermal fluctuations render individual spikes so wide that they overlap and become not clearly discernible. Then, in order to make the examination of CO spikes possible, we were compelled to choose $T_{\min} \approx T_{sg}/4$ in our simulations.

Figure 6(b) shows the mean overlap distribution $p(q)$ for SC arrays at $T = 0.2$ for three values of $N$. $p(q)$ exhibits two large peaks at $|q| \approx 1$ that correspond to the self overlap of pure states. $p(q)$ is approximately flat in the region of small $q$, with $p(0) \neq 0$ and $p(0)$ essentially independent of $N$, as found for the EA model [41]. This behavior is in conflict with the droplet picture of SG, for which $p(0)$ vanishes in the thermodynamic limit [21].

Plots of $\delta p(q)^2$ versus $q$ are shown for SC arrays at the same temperature in figure 6(c). $\delta p(q)^2$, which is a measure of sample-to-sample fluctuations of $p_J(q)$ from the average $p(q)$, does not change appreciably with $N$. According to the RSB scenario, $p_J(q)$ should exhibit many CO spikes that become Dirac delta functions as $N$ increases, bringing about a diverging $\delta p(q)^2$ in the thermodynamic limit.

\(^4\)This might seem to be in contradiction with the fact that $\xi_4/L$ curves cross, as shown in figures 4(a) and (b), and that, as pointed out in [36], $\xi_4/L$ versus $T$ curves merge, instead of crossing, for the 2D XY model as $T \to T_{sg}$ or $T \to T_{k2}$ from above. Some specific examples in [18] illustrate how both merging and spreading as $T$ decreases below $T_{sg}$ can occur depending on some minor details of $G(r)$.\n
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**Figure 5.** Semilog plots of $\xi_4^2/L^2$ versus $1/L$ for SC systems, and $T = 0.2$ (○), $T = 0.3$ (●), $T = 0.4$ (○), $T = 0.5$ (○), $T = 0.6$ (△), $T = 0.7$ (♦), $T = 0.8$ (○), $T = 0.9$ (○), $T = 1.0$ (●), $T = 1.1$ (■). $T = 1.2$ (▲), and $T = 1.3$ (●). Dashed lines are guides to the eye.

**Figure 6.** (a) Overlap distributions $p_J(q)$ for SC systems with $N = 512$ and $T = 0.2$ for three samples with different realizations of disorder (b) Plots of the averaged distribution $p(q)$ versus $q$ for SC systems with $T = 0.2$ and the values of $N$ shown. (c) The same as in (b) for $\delta p(q)^2$. Similar results were obtained for RCP systems.
Figure 7. (a) Plots of $X^0$ versus $T$ for SC systems, $Q = \frac{1}{4}$ and the values of $N$ indicated in the figure. (b) The same plots for RCP systems. (c) The same plots for the SK model.

Figure 8. (a) Plots of $\Delta^0$ versus $T$ for SC systems, with $Q = \frac{1}{4}$ and the values of $N$ indicated in the figure. (b) The same plots for RCP systems. (c) The same plots for the SK model.

Figure 9. (a) Plots of $g^0$ versus $q$ for SC systems at $T = 0.2$, with $Q = \frac{1}{4}$ and the values of $N$ indicated in the figure. (b) The same plots for RCP systems. (c) The same plots for the SK model at $T = 0.24$. Note that $T \approx T_{sg}/4$ in all three cases.

Figure 10. (a) Plots of $w^0$ versus $T$ for SC systems for $Q = \frac{1}{4}$ and the values of $N$ indicated in the figure. (b) The same plots for RCP systems. (c) The same plots for the SK model.

3.3. Cross overlap spikes

The shape and width of CO spikes from a pair correlation function has been used to study the SG phase of the EA and SK models [42]. We define

$$G^0_J(q) \equiv \int_0^Q d\kappa_2 \int_0^\kappa_2 \delta(\kappa_2 - \kappa_1 - q) p_J(\kappa_1) p_J(\kappa_2),$$

and $G^0(q)$ as the average of $G^0_J(q)$ over samples. We have also computed the normalized function

$$g^0(q) = \frac{G^0(q)}{\int_0^Q G^0(q) \, dq},$$

which is the conditional probability density that $q = \kappa_2 - \kappa_1$, given that $\kappa_1, \kappa_2 \in (0, Q)$. At very low temperatures, $g^0(q)$ could be interpreted as the averaged shape of all CO spikes provided that individual spikes in $p_J(q)$ distributions do not overlap each other [19]. Plots of $g^0$ versus $q$ for $Q = \frac{1}{4}$ and $T = 0.2$ are shown in figures 9(a) and (b) for SC and RCP arrays respectively, and in figure 9(c) for the SK model at $T = 0.24$. $g^0$ curves are sharp and narrow in all cases. Note that curves for RAD systems in figures 9(a) and (b) do not change appreciably with system size. In contrast, $g^0$ curves for SK in figure 9(c) become sharper as $N$ increases. This is expected for the mean-field RSB scenario, in which CO spikes become Dirac delta functions in the thermodynamic limit.
Figure 11. (a) Plots of the cumulative distribution $\Pi^Q_\omega$ versus $z$ for RCP systems, with $Q = \frac{1}{2}$, $T = 0.2$ and the values of $N$ indicated in the figure. (b) The same as in (a) for the cumulative distribution $\Pi^Q_c$.

Given that $g^Q(q)$ is a normalized distribution, we compute its width as $w^Q \equiv 1 / g^Q(0)$ [42]. Plots of $w^Q$ versus $T$ are shown in figures 10(a) and (b) for RADs on SC and RCP arrays respectively. In both cases, $w^Q$ does not change appreciably with $N$, suggesting that the width of CO spikes do not vanish in the thermodynamic limit $N \to \infty$ for temperatures below $T_{sg}$. This $N$-independence is evident in the low $T$ phase of the figure and is compatible with the reasonable expectation that it remains valid for all $T < T_{sg}$ in the $N \to \infty$ limit. Compare this conclusion with the analogous plots for the SK model displayed in figure 10(c). They do indicate a vanishing width (curves actually go like $w^Q \sim N^{-3/2}$) [19], in agreement with the RSB picture.

3.4. Cumulative distributions

Pair correlation functions do not provide information about the heights of CO spikes in the $(Q, Q)$ region. Yucesoy et al [40] have proposed an observable that depends on those heights. They consider the maximum value of $p_{\omega}^Q(q)$ for $q \in (Q, Q)$,

$$\tilde{p}_{\omega}^Q \equiv \max \{ p_{\omega}^Q(q) : |q| < Q \},$$

and count a sample as peaked if $\tilde{p}_{\omega}^Q$ exceeds some specified value $\epsilon$. Then, the cumulative distribution $\Pi^Q_\omega(z)$ of non-peaked samples is computed as a function of $z$. Plots of $\Pi^Q_\omega$ versus $z$ for RAD on RCP arrays are shown in figure 11(a) for $T = 0.2$ and $Q = \frac{1}{2}$. In these plots $\Pi^Q_\omega$ becomes size-independent for $N \geq 216$. In contrast, simulations for the SK model have shown that $\Pi^Q_\omega(z)$ decreases as $N$ increases for $z \gtrsim 0.5$ at low temperatures [19]. The latter is in agreement with the RSB picture, for which CO spikes become Dirac delta functions in the $N \to \infty$ limit.

Following [43], we define the cumulative distribution $\Pi^X_\omega(z)$ of $X^Q_{\omega}$ as the fraction of samples having $X^Q_{\omega} < z$. Semilog plots of $\Pi^X_\omega$ versus $z$ for RCP arrays in figure 11(b) are size independent for large $z$ and follow a power-law behavior for small $z$, similarly to a RSB scenario.

4. Conclusions and discussion

We have studied disordered dense packings of $N$ identical classical Ising dipoles at low temperature. Each dipole is the total magnetic moment of a single-domain spherical NP. The anisotropy in each NP obliges the magnetic moment to lie along a randomly oriented easy axis. For this reason, such packings are called random axis dipole (RAD) systems. We have assumed that the orientations of all dipoles remain frozen, that is, they do not participate in the dynamics.

Two types of dense RAD systems have been considered: (i) the NP placed on the sites of simple cubic (SC) lattices and (ii) random close packings (RCP) that fill the maximum possible volume fraction, $\phi = 0.64$. Such densely packed systems may in principle lie in between the diluted version of the same model (where the coupling values $J$ are distributed as $P(J) \sim J^2$) which has been found to behave marginally, and the EA model where $P(J)$ is dominated by the short range, for which the lower critical dimension is $d_q < 3$. In effect, in dense systems $P(J)$ has a tail decreasing like $1/J^2$ for far away dipoles and a different functional form for nearer dipoles (see figure 1).

From the study of the overlap parameter $q$, the associated correlation length and related observables, we have found a marginal behavior for dense RAD packings on SC and RCP lattices for temperatures below $T_{sg}$. From the dependence of the correlation length $\xi_{\omega}$ on the temperature $T$ and on the system size $N$, we have found $T_{sg} = 0.75(2)$ and $T_{sg} = 0.78(3)$ for SC and RCP lattices respectively. In the SG phase we have observed (i) an algebraic decay of $q_2$ with the number $N$ of dipoles, and (ii) absence of divergences in the ratio $\xi_{\omega}/L$ as a function of $N$ (see section 3.1).

In spite of the existence of a quasi-long-range SG order (like in the 2D XY model), the overlap distributions $p_{\omega}(q)$ are comb-like and markedly sample dependent, as occurs for the Edwards–Anderson and the Sherrington–Kirkpatrick models. We have studied the sample-to-sample statistics of $p_{\omega}(q)$ for $q \in (-Q, Q)$ at low temperatures (section 3.2), finding that $P(q)$ and $\delta p(q)^2$ (as well as $X^Q$ and $\Delta^Q$) do not vary with $N$. By also computing the averaged width $w^Q$ of the spikes found in $p_{\omega}(q)$ distributions (section 3.3), we conclude that $w^Q$ does not vanish in the thermodynamic limit. Accordingly, the fraction of samples with spikes higher than a certain threshold does not change with $N$ at low temperatures (section 3.4).

Altogether, these results are in agreement with the above-mentioned marginal behavior, at least for the relatively modest system sizes considered here. Our findings for densely packed RAD systems resemble the behavior previously observed for systems of Ising dipoles with strong dilution in spite of the fact that the geometry for diluted and dense systems and their distribution of couplings are qualitatively different (see figure 1).

It is worth mentioning that a recent investigation of a random Coulomb antiferromagnet in three dimensions, with interactions falling off as $1/r$ in the large distance limit, also leaves some room for marginal behavior [44].
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