Non-trivial link overlap distribution in three-dimensional Ising spin glasses

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We investigate the distributions of the link overlap, $P(Q)$, in 3-dimensional Ising spin glasses. We use clustering methodology to identify a set of pairs of states from different Gibbs states, and calculate its contribution to $P(Q)$. We find that the distribution over this set does not become trivial as the system size increases.

I. INTRODUCTION

While equilibrium properties of infinite range spin glasses\textsuperscript{2,3,4,5} are completely understood within the framework of replica symmetry breaking (RSB)\textsuperscript{6,7,8}, spin glasses with short range interactions are the subject of considerable debate and controversy. Open questions address the nature of the low temperature phases\textsuperscript{9,10,11,12} and their theoretical description. Resolution of these issues by experiments or simulations is hindered by the extremely long relaxation time required for equilibration.

The Edwards-Anderson model is the most widely studied type of short-range Ising spin glass

\begin{equation}
H(s) = \sum_{(i,j)} J_{ij} s_i s_j ,
\end{equation}

where the sum is over nearest neighbor sites, $(i,j)$, of a simple (hyper) cubic lattice with periodic boundary conditions, $s_i = \pm 1$, and the couplings, $J_{ij}$, are independent random variables taken from a normal distribution with zero average and standard deviation $J = 1$. For the infinite range Sherington Kirkpatrick (SK) model the sum in Eq. 1 is over all pairs of sites and $J = 1/\sqrt{N}$.

The system (in 3 or more dimensions) has a finite critical temperature. Recent numerical analysis of 3-dimensional Ising spin glasses (3DISG) yielded $T_c = 0.951(9)$, whereas for the SK model $T_c = 1$. The high temperature phase of the model is a disordered paramagnet. As the temperature decreases below $T_c$ the system undergoes a transition into a frozen spin-glass phase.

In the spin glass phase, the microstates are divided into Gibbs states; each constitutes an ergodic subset of phase space, i.e. a maximal subspace that the system can span (or visit) as time tends to infinity. In a finite system phase space consists of one such state; however, we identify the infinite volume Gibbs states with subsets of the phase space surrounded by free energy barriers, whose height diverges as $N \rightarrow \infty$. Here the term “Gibbs states” refers to such subsets.

Extensive recent numerical investigations, done at finite $T$\textsuperscript{13,14,15,16}, as well as ground state analysis\textsuperscript{13,14,15,16}, suggest evidence for a multiplicity of Gibbs states in the low temperature phase of the 3DISG. The most widely measured properties are

\begin{equation}
q(s, t) = N^{-1} \sum_{i=1}^{N} s_i t_i ,
\end{equation}

the site overlap between any two microstates $s$ and $t$, the global distribution of $q$,

\begin{equation}
p_q(q) = Z^{-2} \sum_{s} e^{-H(s)} \sum_{t} e^{-H(t)} \delta(q(s, t) - q) ,
\end{equation}

and, in particular, $p(q) = \overline{p_q(q)}$, the distribution averaged over the random variables $\{J_{ij}\}$. In [3] $Z$ is the partition function of the system.

There is general agreement that in 3DISG the averaged distribution $p(q)$ is not trivial (that is, does not converge to a $\delta$-function in the infinite volume limit) and is not self averaging, in agreement with RSB theory.

As to the droplet theory\textsuperscript{17,18}, although its common interpretation involves a trivial $p(q)$\textsuperscript{19}, it explicitly predicts only the triviality of the local $p(q)$ - the overlap distribution over a finite (large) window in an infinite system. That is, locally there is only one Gibbs state for the system (up to a spin-flip symmetry), so that when a finite window of an infinite system is viewed, the system will be almost always in this Gibbs state.

In order to test this prediction numerically, one should observe the site overlap in a finite constant window as the system size increases\textsuperscript{20}. An alternative is to measure the link overlap

\begin{equation}
Q(s, t) = N_b^{-1} \sum_{(i,j)} s_i s_j t_i t_j ,
\end{equation}

summing over all the $N_b$ bonds in the system, e.g. over all nearest neighbors pairs in the case of 3DISG. The distribution of the link overlap, $P_f(Q) = \delta(Q(s, t) - Q)$, is defined similarly to $p_d(q)$ in Eq. 3. The average over realizations is $P(Q) = \overline{P_f(Q)}$.

According to the droplet theory $P(Q)$ is trivial and consequently $P_f(Q) = P(Q)$. This was predicted earlier from scaling analysis of numerical results\textsuperscript{20,21}. Newman and Stein\textsuperscript{22,23} showed that triviality of $P(Q)$ for given boundary conditions may be deduced from general considerations even if one relaxes some of the scaling assumptions of the droplet theory. However, according to
we produced a weighted sample of microstates. We used
in each inter-temperature step the transition probability

teratures, \( N \) and their values were determined so that
so that in each inter-temperature step the transition probability

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\[ P(Q) = \text{Prob}(Q(s,t) = Q | s,t \in G_1) \]  

- the distribution of overlaps within \( G_1 \) - which is trivial in the thermodynamic limit. At small system sizes, as the ones considered in this work, the peak of \( P_1(Q) \) is still wide, and it narrows as \( L \) increases. Since even at finite (albeit low) temperatures \( P_1(Q) \) dominates the distribution, one would expect a clear decrease of the variance of \( P(Q) \) with size, as observed in Fig. 1, even if \( P(Q) \) is non-trivial in the thermodynamic limit. Hence decrease of the second moment of the distribution with size may capture nothing but the narrowing of the dominant single peak part of a non-trivial \( P(Q) \); in order to test non-triviality, it is much more effective to measure the size dependence of a quantity which is independent of the dominant (but uninformative) \( P_1(Q) \).

We present \( P(Q) \) in Fig. 3(a) for two temperatures, one above and one below \( T_c \), for three system sizes. Above \( T_c \), \( P(Q) \) consists of a single peak which narrows as the \( L \) increases; approaching \( \delta(Q - \langle Q \rangle) \). Below \( T_c \) the distribution consists of a dominant peak, whose main contribution comes from \( P_1(Q) \), and a tail at lower values of \( Q \). As \( L \) increases, the peak narrows and since the weight of the peak is much larger then that of the tail, a single measured parameter (say moment) may reflect mainly the convergence of the peak to a \( \delta \) function, which is expected irrespective of whether \( P(Q) \) is trivial or not. To address this question one has to assess whether the weight of the tail of \( P(Q) \), say, in the range \( 0 \leq Q \leq 0.8 \), decreases with increasing system size.

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modynamic limit, it must originate from pairs of microstates that belong to different Gibbs states. Ideally, we would like to calculate the link overlap distribution over all such pairs. In finite systems this is not possible since we cannot identify the Gibbs states unambiguously. However, the coarsest partitions of phase space can be observed clearly, even for very small systems.\(^{12,16}\) This partition consists of two sets of microstates, \( C_1 \) and \( C_2 \), which we identify by the average linkage agglomerative clustering algorithm.\(^{30}\)

The statistical weights of the sets \( C_1 \) and \( C_2 \) remain finite as the system size increases, and the average site
overlap between them remains different from the overlap between two microstates that belong to the same set\(^{12}\). Therefore the contribution of the set of pairs of microstates \(\{ (s,t) \mid s \in C_1, t \in C_2 \} \) to \(P(Q)\) remains finite as the system size increases.

Following the method described in Ref. \(^{29}\) for \(p(q)\), we define

\[
P_o(Q) = \text{Prob}(Q(s,t) = Q \mid s \in C_1, t \in C_2).
\]

In order to move from a state in \(C_1\) to a state in \(C_2\), some groups of spins (domains) have to be flipped. We refer to the surfaces that separate these flipped domains from spins that did not flip as domain walls. If these domain walls have a vanishing density, the fraction of links affected by switching one micro-state from \(C_1\) to \(C_2\) goes to zero as the system size increases, and hence at the thermodynamic limit we will have \(P_o(Q) = P(Q)\).

In Fig. \(^3\)(a) we observe that for 3DISG at \(T = 0.28J/k_B\), \(P(Q)\) seems to converge to a peak at \(Q \simeq 0.9\). If \(P_o(Q)\) does not converge to the same distribution, we expect it to have a non-vanishing weight at \(Q < 0.9\). We calculate \(\int_0^{0.8} P_o(Q) dQ\). For \(L = 8, 10, 12\) the values of the integral are 0.81(5), 0.83(4), 0.80(4) respectively, suggesting that the weight of \(P_o(Q)\) for \(0 \leq Q \leq 0.8\) does not decrease. Thus, \(P_o(Q)\) does not converge to the peak at \(Q \simeq 0.9\) which dominates \(P(Q)\).

These results imply that the domain walls between \(C_1\) and \(C_2\) occupy a finite fraction of the volume of the system. Since \(C_1\) and \(C_2\) remain finite and distinguishable as the system size increases\(^{12}\), \(P_o(Q)\) (shown in Fig. \(^3\)(b)) constitutes a finite contribution to \(P(Q)\). Consequently, \(P(Q)\) is not trivial at the thermodynamic limit.

FIG. 3: (a) The link overlap distribution measured for 3DISG systems at \(T = 0.28J/k_B < T_c\), in linear plot and linear-log plot (inset). (b) The distribution \(P_o(Q)\) for \(T = 0.28J/k_B\), which gives a finite contribution to \(P(Q)\). All distributions are normalized to unity. The grey lines above and below each curve indicate the error range.

IV. DISCUSSION

According to RSB theory, \(P(Q)\) is not trivial. More over, all overlap measures are equivalent\(^{23,31}\), so \(Q\) is determined by the value of the site overlap \(q\). This statement is trivial for the SK model, where the sum in Eq. \(^1\) is over all pairs of sites, so \(Q(s,t) = q^2(s,t) - N^{-1}/(1 - N^{-1})\). In 3DISG the site overlap and bond overlap have different roles: given two states of the system, the site overlap is given by the volume of spin-domains flipped between the states, and the link overlap by the surface area of the domain walls.

Recent numerical investigation of 3DISG systems\(^{25}\) indicated that the two overlaps are equivalent. This result along with previous numerical evidence for the non-triviality of the site overlap, \(p(q)\), yield a non-trivial \(P(Q)\) and support the results presented here.
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