Statistics of lowest excitations in two dimensional Gaussian spin glasses

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A detailed investigation of lowest excitations in two-dimensional Gaussian spin glasses is presented. We show the existence of a new zero-temperature exponent \(\theta\) describing the relative number of finite-volume excitations with respect to large-scale ones. This exponent yields the standard thermal exponent of droplet theory \(\theta\) through the relation, \(\theta = d(\lambda - 1)\). Our work provides a new way to measure the thermal exponent \(\theta\) without any assumption about the procedure to generate typical low-lying excitations. We find clear evidence that \(\theta < \theta_{DW}\) where \(\theta_{DW}\) is the thermal exponent obtained in domain-wall theory showing that MacMillan excitations are not typical.

Despite three decades of work in the field of spin glasses major issues such as their low-temperature behavior still remain unresolved. One of the main achievements has been a good understanding of mean-field theory which nevertheless does not include spatial effects which manifest as droplet excitations. Leaving aside the controversy whether replica symmetry breaking is or not a good description of the spin-glass phase, it is reasonable to expect that a phenomenological approach to the spatial structure of lowest excitations should satisfactorily account for their low-temperature properties. McMillan proposed that thermal properties in spin glasses are determined by the scaling behavior of the typical largest excitations present in the system. Therefore, he assumed that the energy cost of large scale excitations of length \(L\) scales like \(L^\theta\), \(\theta\) being the thermal exponent. Using domain-wall renormalization group ideas he also introduced a practical way to determine the leading energy cost of low-lying large-scale excitations. It consisted in measuring the energy defect of a domain-wall spanning the whole system obtained by computing the change of the ground state energy when switching from periodic to anti periodic boundary conditions in one direction. This idea has been further elaborated and extended to deal with equilibrium and dynamical properties of spin glasses in a scenario nowadays referred as droplet model. Several works have used McMillan’s method to determine the value of \(\theta\) in two and three dimensions.

The purpose of this work is to show an alternative approach to determine the low \(T\) behavior of spin glasses by studying the size and energy spectrum of the lowest excitations by introducing two exponents (\(\lambda\) and \(\theta'\)) needed to fully characterize the zero-temperature fixed point. The \textit{entropic} exponent \(\lambda\) describes the probability to find a large-scale lowest excitation spanning the whole system, while the exponent \(\theta'\) describes the system-size dependence of the energy cost of this excitation.

The underlying theoretical background of our approach is the following. To investigate the leading low-temperature behavior in spin glasses let us consider expectation values for moments of the order parameter by keeping only the ground state and the first excitation. This approach was introduced \(^{(4)}\) and can be extended to higher-order excitations to construct a low-temperature expansion for spin glasses \(^{(5)}\). This is described in detail in a separate publication \(^{(6)}\). For simplicity, here we restrict the analysis to the first linear expansion in \(T\) by keeping only the first excitation. If \(q = \{\sigma, \tau\}\) denotes the overlap between two replicas (i.e. configurations of different systems with the same realization of quenched disorder) then the expectation value \(\langle q^2 \rangle\) can be written as follows:

\[
\langle q^2 \rangle = 1 - \frac{2}{V^2} \sum_v \int_0^\infty dE P(v, E) v (V - v) \text{sech}^2 \left( \frac{E}{2T} \right),
\]

where \(P(v, E)\) is the joint probability distribution to find a sample (among an ensemble of \(N_s\) samples) where the lowest excitation has \(v\) spins overturned respect to the ground state (so the overlap between the ground and that excited state is \(q = 1 - 2v/V\), \(V\) being the total volume of the system) and with energy cost or gap \(E\). If \(v_s\) and \(E(s)\) denote the volume and excitation energy of the lowest excitation for sample \(s\) then,

\[
P(v, E) = \frac{1}{N_s} \sum_{s=1}^{N_s} \delta(v - v_s) \delta(E - E(s)).
\]

Using the Bayes theorem this joint probability distribution can be written as \(P(v, E) = g_v \tilde{P}_v(E)\) where \(\sum_{v=1}^{V} g_v = \int_0^\infty dE \tilde{P}_v(E) = 1\), the last equality being valid for any \(v\). \(g_v\) is the probability to find a sample such that its lowest excitation has volume \(v\) and \(\tilde{P}_v(E)\) is the conditioned probability for this excitation to have a gap equal to \(E\). A simple low-temperature expansion of \(\tilde{P}_v(E)\) up to linear order in \(T\) yields,

\[
\langle q^2 \rangle = 1 - \frac{4T}{V^2} \sum_{v=1}^{V} g_v \tilde{P}_v(0) v (V - v)
\]

showing that the leading behavior is determined by both the \(g_v\) and the density of states at zero gap \(\tilde{P}_v(0)\). In the droplet model it is generally assumed that typical
lowest excitations have average volume \( \overline{v} = \sum_v v g_v \) diverging with \( V = L^D \) and density weight at zero gap \( \tilde{P}_v(0) \sim 1/L^\theta \) where \( \theta \) is the thermal exponent. In principle, a single exponent \( \theta \) describes the scaling behavior of large-scale excitations with volume \( v \propto V \) which are supposed to determine the zero-temperature critical behavior. Actually, assuming that \( g_I/g_V \sim O(1) \), eq. (3) suggests that the contribution of small-scale excitations to the sum in the r.h.s would be negligible in the large \( V \) limit. Under these reasonable assumptions one obtains \( <q^2> = 1 - c \ell / L^\ell \), where \( c \) is a non-universal stiffness constant related to the particular model. Our purpose here is to show that \( g_I/g_V \) diverges in the large \( V \) limit in such a way that the contribution of small-scale excitations to the r.h.s of (3) is as important as the contribution of the large-scale ones, thus leading to a new physical meaning of the thermal exponent \( \theta \).

![Fig. 1](image)

**FIG. 1.** \( g(q) \) versus \( 1-q \) for the PP (left panel) and FF case (right panel) for different lattice sizes \( L = 5 - 11 \) (PP) and \( L = 6 - 16 \) (FF) from top to bottom. In both insets we plot the scaling function \( g(q)V^\lambda \) vs \( 1-q \) with \( \lambda = 0.7 \).

Several numerical works have recently searched for low-lying excitations in spin glasses using heuristic algorithms. But, to our knowledge, no study has ever presented exact results about the statistics of lowest excitations. In this paper we have exactly computed ground states and lowest excitations in two-dimensional Gaussian spin glasses defined by

\[
\mathcal{H} = -\sum_{ij} J_{ij} \sigma_i \sigma_j
\]

where the \( \sigma_i \) are the spins \((\pm 1)\) and the \( J_{ij} \) are quenched random variables extracted from a Gaussian distribution of zero mean and unit variance. These have been computed by using a transfer matrix method working in the spin basis. Representing each spins state by a weight and a graduation in the energy we can build explicitly the ground state by keeping the largest energy and next by iteration the first excitation and so on. The continuous values for the couplings assures that there is no accidental degeneracy in the system (apart from the trivial time-reversal symmetry \( \sigma \rightarrow -\sigma \)). Calculations have been done in systems with free boundary conditions in both directions (FF), periodic boundary conditions in both directions (PP) and free boundary conditions in one direction but periodic in the other (FP). In all cases we find the same qualitative and quantitative results indicating that we are seeing the correct critical behavior.

We found ground states and lowest excitations for systems ranging from \( L = 4 \) up to \( L = 11 \) for FF and up to \( L = 16 \) for PP and FF. The number of samples is very large, typically \( 10^6 \) for all sizes. This requires a big amount of computational time and calculations were done in a PC cluster during several months. For each sample we have evaluated the volume of the excitation \( v \) (and hence the overlap \( q = 1 - 2v/V \) between the ground state and the first excitation) and the gap \( \lambda \). From these quantities we directly obtain \( g_v \) and \( \tilde{P}_v(\lambda) \). In figure 1 we show \( g(q) = \frac{V}{g_v} \) as function of \( q \) for different sizes in the PP and FF cases. We can clearly see that there are excitations of all possible sizes but the typical ones which dominate by far are single spin excitations. To have a rough idea of the number of rare samples giving large scale excitations let us say that nearly half of the total number of samples have one-spin lowest excitations, whereas less than 10% of the samples have lowest excitations with overlap \( q \) in the range 0–0.5. This disparity increases systematically with size. A detailed analysis of the shape of \( g_v \), reveals that it has a flat tail for large-scale excitations and a power law divergence for finite-volume excitations. The \( g_v \) can be excellently fitted by the following scaling form,

\[
g_v = \frac{G(q)}{V^{\lambda+1}} = \frac{1}{V^{\lambda+1}} \left( A + \frac{B}{(1-q)^{\lambda+1}} \right) . \tag{5}
\]

This type of scaling, applied only to large-scale excitations, was proposed in. Although we do not have a simple explanation for \( (3) \) we emphasize how such expression interpolates extremely well the whole spectrum of sizes matching the two volume sectors: a small-scale sector \((\text{finite } v)\) \( g_v \sim 1/V^{\lambda+1} \) and a large-scale sector \((\text{finite } v)\) \( g_v \sim 1/V^{2\lambda+1} \). This matching explains why there is a unique exponent \( \lambda \) in \( (3) \) which describes two completely different volume sectors. Note that although the \( g_v \) is defined for discrete volumes, in the limit \( V \gg 1 \) values of \( q \) are equally spaced by \( \Delta q = 2/V \) and the function \( g(q) = \frac{V}{2} g_v \) becomes continuous if expressed as function of \( q \) instead of the integer variable \( v \),

\[
g(q) = \frac{1}{2V^\lambda} \left( A + \frac{B}{(1-q)^{\lambda+1}} \right) . \tag{6}
\]

Although eq. (5) diverges for \( q = 1 \) apparently leading to a violation of the normalization condition for the \( g_v \), it must be emphasized that no excitation has \( q = 1 \) so there is a maximum cutoff value \( q^* = 1 - 2/V \) corresponding to one-spin excitations. The normalization condition for the \( g(q) \) using \( (3) \) yields in the large \( V \) limit,

\[
\int_{0}^{q = 1 - 2/V} g(q) dq = 1 \rightarrow A - \frac{B}{2V^\lambda} + \frac{B}{2^{\lambda+1}} = 1 \tag{7}
\]
implying \( \lambda \geq 0 \). The divergent term \( (q \to 1) \) in (6) shows that one-spin excitations dominate the whole spectrum. In fact, \( g(1) \approx O(1) \gg g(V/2) \approx 1/V^{\lambda+1} \) so that the majority of excitations are finite-volume excitations. But the average excitation volume \( \bar{v} = \frac{\sum v_{\text{exc}}}{N} \approx A V^{1-\lambda} \) diverges in the \( V \to \infty \) limit and differs from the typical excitation volume \( v_{\text{typ}} \approx 1 \). This yields an independent measurement of the exponent \( \lambda \). By fitting the average volume to the expression \( \bar{v} = C_1 + C_2 V^{1-\lambda} \) or by measuring the ratio \( g(V/2)/g(1) \approx D_1 + D_2 V^{1-\lambda} \) we get an effective exponent \( \lambda_{\text{eff}} = 0.7 \pm 0.05 \) as best fitting value. Although we find some systematic corrections in the value of \( \lambda \), our results are compatible with the general equation (6) plus some systematic subleading corrections. We will see later how we can obtain a better estimate of \( \lambda \).

\[
\hat{V}_{\text{eff}} \propto V^{1-\lambda}\]

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FIG. 2. Gap distribution \( P(E) \) vs \( E \) for different lattice sizes in the PP case. In inset a) Scaling obtained from the ansatz (8) with \( \theta'_{\text{eff}} = -1.6 \). In inset b) we show the \( \hat{P}_v(E) \) for different excitation sizes \((q = 0.5, q = 0)\) for a lattice size \( L = 10 \). Note that the distribution is independent of the size of the excitation.

After having discussed the \( g_v \) we show the results for the energy gap distribution \( \hat{P}_v(E) \). In figure 3 we show this distribution for the PP case. Similar results are obtained for the FF and FP cases. Quite remarkably, this distribution does not depend on the size \( v \) of the excitation, hence both large and small-scale excitations are described by the same gap distribution (inset b) of figure 2). The normalized \( \hat{P}_v(E) \) has the following scaling behavior,

\[
\hat{P}_v(E) = L^{-\theta'} P\left(\frac{E}{L^{\theta'}}\right)
\]

Since both the exponent \( \theta' \) and the scaling function \( P \) are independent of \( v \) this implies that the gap probability distribution \( P(E) = \sum_{v \geq 1} g_v \hat{P}_v(E) \) satisfies the same scaling behavior (8). In the inset a) of figure 2 we also show the best data collapse for \( P(E) \) obtained with an effective exponent \( \theta'_{\text{eff}} \approx -1.6 \). A detailed study of the moments of \( P(E) \) computed for different values of \( L \) shows that there are also strong sub dominant corrections to the leading scaling (8) and that the value which gives the best data collapse turns out to be \( \theta' = -1.7 \pm 0.1 \). We will argue below that, for Gaussian couplings, \( \theta' \leq -2 \) and explain why finite-size effects are so big.

Now we want to show how the exponents \( \lambda \) and \( \theta' \) combine to give the usual scaling exponent \( \theta \) describing the energy cost of typical thermal excitations in droplet theory. One of the most relevant results from the ansatz in (6) is that both small and large scale excitations contribute to low-temperature properties. In general, let us consider any expression (such as (8)) involving a sum over all possible volume excitations. Restricting the sum to the large-scale regime \( (v/V \) finite) the net contribution to such sum is proportional to \( V g_v \hat{P}_v(0) \approx L^{-\theta' - d\lambda} \). Coming back to (8) we note, using (8), that both small and large-scale excitations yield a contribution of the same order \( TL^{-\theta' - d\lambda} \). This is a consequence of the aforementioned fact that there is a single exponent \( \lambda \) describing the large and small sectors of the volume spectrum (8). These considerations lead to the existence of an exponent \( \theta = \theta' + d\lambda \) determining the zero-temperature critical behavior of the order parameter \( < q^2 > \). Because of the systematic corrections in the values of the exponents \( \lambda \) and \( \theta' \), in principle it is difficult to give an accurate estimate for the exponent \( \theta \). Nevertheless, despite of these strong corrections, the combination \( \theta = \theta' + d\lambda \) seems to be very stable (see figure 3). Thus we computed, for each size, the combination

\[
A(L) = L^{\frac{\bar{v}(L)}{\bar{v}(0)}}
\]

Since \( \bar{v}(L) \approx L^{\theta'} \) and \( \bar{v}(L) \approx L^{\theta(1-\lambda)} \), then the fit of \( A(L) \) gives a direct estimate of \( \theta(L) = \theta(L) + d\lambda(L) \). In Fig. 3 we show the effective exponent form a fit of \( A(L) \) vs. \( L \), with data in the range \([L, \cdots, L_{\text{max}} = 11]\) for PPBC. We also show for comparison the effective exponent for \( \theta_{\text{DW}} \) obtained also with PPBC. Our best values for \( \theta \) is \(-0.46(1)\) for the PPBC. This value is very close to the finite-temperature (Monte Carlo or transfer matrix) estimates \( \theta = 0.48(1) \) but certainly smaller than domain-wall calculations \( \theta_{\text{DW}} = -0.28(2) \). Since our estimate for \( \theta \) has been obtained with a new independent method it clearly shows that \( \theta \neq \theta_{\text{DW}} \).

Now we come back to the issue why in the large volume limit \( \theta' \) should converge to a value \( \leq -d \). The argument (6) goes as follows. Consider the ground state and all possible one-spin excitations. Because one-spin excitations are not necessarily the lowest excitations the statistics of the lowest one-spin excitations must yield a upper bound \( \theta'_0 \) for the value of \( \theta' \), i.e. \( \theta' \leq \theta'_0 \). The statistics of the lowest one-spin excitations is determined by the behavior of the ground-state local field distribution \( P(h) \) in the limit \( h \to 0 \). If \( P(h) \) is self-averaging and \( P(0) \) is finite in the large size limit then the statistics of the lowest excitations must be governed by the exponent \( \theta'_0 = -d \). Numerical results in 2 dimensions show that the aforementioned conditions are clearly satisfied indicating that.
the typical low-lying excitations and our approach offers a new and independent way to estimate the thermal exponent $\theta$ without the need to generate typical low-lying excitations. Although we have focused our research in the two-dimensional Gaussian spin glass we believe that our conclusions remain valid for general dimensions beyond $d = 2$.

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