

LETTER TO THE EDITOR

Scaling approach to order parameter fluctuations in disordered frustrated systems

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Abstract

We present a constructive approach to obtain information about the compactness and shape of large-scale lowest excitations in disordered systems by studying order parameter fluctuations (OPF) at low temperatures. We show that the parameter G that measures OPF is $1/3$ at $T = 0$ provided the ground state is unique and the probability distribution for the lowest excitations is gapless and with finite weight at zero excitation energy. We then apply zero temperature scaling to describe the energy and volume spectra of the lowest large-scale excitations that scale with the system size and have a weight at zero energy $\hat{P}_v(0) \sim l^{-\theta'}$ with $v = l^d$. A low-temperature expansion reveals that, OPF vanish like $L^{-\theta}$, if $\theta > 0$ and remain finite for space-filling lowest excitations with $\theta = 0$. The method can be extended to extract information about the shape and fractal surface of the large-scale lowest excitations.

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1. Introduction

There is a long-standing controversy on the nature of low-temperature excitations in spin glasses. This discussion has seen a strong revival in the last years due to the large increase of computational capabilities together with the simultaneous development of more refined and powerful numerical techniques [1, 2]. These have largely improved the ability to find exact ground states or to equilibrate small systems at very low temperatures. The aim of this letter is to present some analytical results on this subject by investigating order parameter fluctuations (hereafter denoted by OPF) and showing how they can give us information about the topology of the excitations in spin glasses.

The study of parameters measuring OPF has been proven to be very powerful at locating finite temperature phase transitions in disordered systems [3, 4]. Recent studies [5] show that these parameters can also divulge information about the frozen phase and thus shed some light on the nature of the spin glass phase. The introduction of G was originally motivated by the existence of the well known Guerra sum rules for spin glasses [6], and in particular the following

one: $\overline{\langle q^2 \rangle^2} = \frac{1}{3} \overline{\langle q^4 \rangle} + \frac{2}{3} \overline{\langle q^2 \rangle}^2$ where $q = \frac{1}{V} \sum_{i=1}^V \sigma_i \tau_i$ is the usual overlap between different replicas $\{\sigma, \tau\}$, $\langle \dots \rangle$ and $\overline{\langle \dots \rangle}$ stand for thermal and disorder averages, respectively. This relation implies that in systems with non-vanishing OPF in the frozen phase, the parameters G and A defined as

$$G = \frac{\overline{\langle q^2 \rangle^2} - \overline{\langle q^2 \rangle}^2}{\overline{\langle q^4 \rangle} - \overline{\langle q^2 \rangle}^2} \quad A = \frac{\overline{\langle q^2 \rangle^2} - \overline{\langle q^2 \rangle}^2}{\overline{\langle q^2 \rangle}^2} \quad (1)$$

have the following behaviour in the infinite volume limit: $G = \frac{1}{3} \theta (T_c - T)$ and $A \equiv \hat{A}(T)$ is a non-vanishing function of T (this result for A being evidence of replica symmetry breaking (RSB)).

Very recently it was conjectured in [7] (henceforth referred to as RS) that for systems of Ising variables, G takes the universal value $1/3$ at $T = 0$ for finite volume systems under two mild assumptions: the uniqueness of the ground state and the absence of a zero gap in the local field distribution. In RS the main scenarios for OPF were discussed and many examples were given to check the validity of such a conjecture. Moreover, the conjecture was proven for finite volume systems provided that the limit $T \rightarrow 0$ is taken before the limit $V \rightarrow \infty$ by showing that one-spin excitations with finite probability at zero local field yield at low temperature the dominant (linear in T) contribution to OPF.

In this letter we prove that these results generally hold whatever the size of the lowest excitations is, provided these are gapless and have finite weight at zero excitation energy. Moreover, we will obtain valuable information about the size of the excitations by considering the low-temperature behaviour of the OPF parameters. In particular, we will see how we can establish a scaling theory for the lowest large-scale excitations that relates OPF to the $T = 0$ thermal scaling exponent θ' and the exponent that characterizes the distribution of large-volume excitations γ . We exemplify these findings in the spin glass chain. In this letter we analyse the excitations through the overlap parameter q and we do not discuss the shape of the excitations, an issue which will be addressed by studying the energy overlap or link overlap order parameters in a similar way.

2. The model

Consider a system of V Ising spins with a general Hamiltonian

$$\mathcal{H} = - \sum_{i,j} J_{ij} \sigma_i \sigma_j \quad (2)$$

where the J_{ij} are the quenched variables. In general these can be either 0 (depending on the dimensionality and interaction range of the system) or distributed according to some continuous $P(J)$. For a continuous distribution of couplings there is a unique ground state (up to a global flip of all the spins), whose configuration we denote by $\{\sigma_i^*\}$. This Hamiltonian can be rewritten in terms of local fields, following the formulation given in RS, $\mathcal{H} = - \sum_i \sigma_i h_i$. In the ground-state configuration each spin σ_i is aligned with its local field h_i , so that the ground-state energy is $E_{GS} = - \sum_i \sigma_i^* h_i^* = - \sum_i |h_i^*| = - \sum_{i,j} J_{ij} \sigma_i^* \sigma_j^*$. Suppose that for a given sample we know the ground-state configuration $\{\sigma_i^*\}$. In this state, we will take the convention that all the spins have the same colour, say red. Consider now a cluster excitation of volume v . In this new state, v spins will change their orientation with respect to the ground-state configuration so that they have a different colour, say blue. Thus, in the excited state the spins will fall into two groups: the red one, which we denote by $\mathcal{D}$; and the blue one, which we denote by $\overline{\mathcal{D}}$. This minimum cost excitation is always a cluster excitation in the sense that all excited spins are connected to each other by bonds. An excitation consisting of two or more disconnected

clusters will necessarily cost more energy than that of reverting one single cluster. Since we are considering a cluster excitation, we can define among these two regions the surface of the excitation or droplet: $\delta\mathcal{D}$. $\delta\mathcal{D}$ will be composed of those pairs of spins of different colour that are connected to each other by at least one bond. Thus the surface contains red ($\delta\mathcal{D} \cap \mathcal{D}$) and blue spins ($\delta\mathcal{D} \cap \bar{\mathcal{D}}$).

The energy cost of such an excitation will depend exclusively on the bonds that connect spins of different colours, defining the surface of the droplet. Therefore, the energy cost reads,

$$\Delta E = 2 \sum_{\substack{i,k \text{ diff. colour} \\ (i,k) \in \delta\mathcal{D}}} J_{i,k} \sigma_i^* \sigma_k^* \quad (3)$$

where each coupling is counted only once. It follows that the lowest excitation with energy (ΔE^*) will correspond to breaking a subset of bonds among the $\{J_{i,k}\}$ such that the value in (3) is minimum.

3. Analysis of OPF fluctuations

If we are at a very low temperature the main contribution to the partition function arises from the lowest excitation. In this limit the partition function reads

$$\mathcal{Z} = e^{-\beta E_{\text{GS}}} (1 + e^{-\beta \Delta E^*}). \quad (4)$$

The computation of the terms involved in G is done following the same procedure used in RS. Different quantities that enter in the definition of G can be expressed in terms of the two- and four-point correlation functions by defining the following objects, $T_{ij} \equiv \langle \sigma_i \sigma_j \rangle^2$ and $T_{ijkl} \equiv \langle \sigma_i \sigma_j \sigma_k \sigma_l \rangle^2$.

$$\langle q^2 \rangle = \frac{1}{V} + \frac{1}{V^2} \sum_{i \neq j} T_{ij} \quad \langle q^4 \rangle = \frac{3}{V^2} - \frac{2}{V^3} + \left(\frac{6V-8}{V^4} \right) \sum_{i \neq j} T_{ij} + \frac{1}{V^4} \sum_{(i,j,k,l)} T_{ijkl}. \quad (5)$$

To compute the two-point correlation functions $\langle \sigma_i \sigma_j \rangle$ we must take into account two different contributions which we denote as U_{ij} and V_{ij} :

- Pairs of spins of the same colour, either blue $\sigma_{i(j)} = -\sigma_i^*$, or red $\sigma_{i(j)} = \sigma_i^*$, both yield the same contribution $\langle \sigma_i \sigma_j \rangle = \sigma_i^* \sigma_j^* \equiv U_{ij}$.
- Pairs of spins having different colours yield $\langle \sigma_i \sigma_j \rangle = \sigma_i^* \sigma_j^* \tanh\left(\frac{\beta \Delta E^*}{2}\right) \equiv V_{ij}$.

In the same way the four-point correlation functions $\langle \sigma_i \sigma_j \sigma_k \sigma_l \rangle$ can be computed by adding two types of contributions: U_{ijkl} and V_{ijkl} .

- When either all four spins have the same colour or there are two spin pairs with different colours, $\langle \sigma_i \sigma_j \sigma_k \sigma_l \rangle = \sigma_i^* \sigma_j^* \sigma_k^* \sigma_l^* \equiv U_{ijkl}$.
- When three spins have the same colour and the other spin has a different colour, $\langle \sigma_i \sigma_j \sigma_k \sigma_l \rangle = \sigma_i^* \sigma_j^* \sigma_k^* \sigma_l^* \tanh\left(\frac{\beta \Delta E^*}{2}\right) \equiv V_{ijkl}$.

The next step in order to compute $\overline{\langle q^2 \rangle}$, $\overline{\langle q^2 \rangle^2}$ and $\overline{\langle q^4 \rangle}$ is to take into account the degeneration d_v of each kind of contribution. This number will depend on the size of the excitation (v). Consider, for instance, the term $\sum_{i \neq j} T_{ij}$. An excitation with v blue spins and $(V-v)$ red ones contributes to T_{ij} with the following degenerations:

- The number of pairs of spins that in the excited state are both red ($d_v = (V-v)(V-v-1)$) or both blue ($d_v = v(v-1)$) yield $U_{ij}^2 = 1$.
- The number of pairs of spins with different colours ($d_v = 2(V-v)v$) yield $V_{ij}^2 \equiv R \equiv \tanh^2\left(\frac{\beta \Delta E^*}{2}\right)$.

Adding all contributions we finally obtain: $\sum_{i \neq j} T_{ij} = (V - v)(V - v - 1) + v(v - 1) + 2(V - v)vR$. Up to now we have contented ourselves with computing the correlation functions but we have not made any hypothesis on the probability distribution of having an excitation of certain volume (v) and energy cost (ΔE^*). When performing the average over the disorder, we have to bear in mind that each sample may have a lowest excitation of size v and energy ΔE^* , yielding a distribution of the lowest excitation energies for every size v . Since there may exist correlations among fields that enhance clusters of certain sizes we make the assumption that excitations of volume v ($< V$) can take place with a finite probability g_v ($\sum_v g_v = 1$) and the energy cost of these excitations at fixed volume v is distributed according to some normalized continuous $\hat{P}_v(\Delta E^*)$, which is only defined for positive ΔE^* . Through these considerations we obtain the following general expression: $\sum_{i \neq j} \bar{T}_{ij} = \sum_{v=1}^{V-1} g_v [V(V - 1) + 2v(v - V) + 2(V - v)v \bar{R}_v^1]$, where $\bar{R}_v^k = \int d\Delta E^* \hat{P}_v(\Delta E^*) (\tanh(\frac{\beta \Delta E^*}{2}))^{2k}$.

In a similar way we can evaluate all terms entering in (5). After some algebra we obtain for the numerator (N) and denominator (D) of G the following expressions,

$$N = \frac{4}{V^4} \left[\sum_v g_v (1 - 2\bar{R}_v^1 + \bar{R}_v^2) v^2 (v - V)^2 - \left(\sum_v g_v (\bar{R}_v^1 - 1) v (V - v) \right)^2 \right] \quad (6)$$

$$D = \frac{4}{V^4} \left[\sum_v g_v (1 - \bar{R}_v^1) 2v^2 (v - V)^2 - \left(\sum_v g_v (\bar{R}_v^1 - 1) v (V - v) \right)^2 \right]. \quad (7)$$

Note that these expressions are invariant under the change $v \rightarrow V - v$ as it should be (for every excitation there is the corresponding one related by time-reversal symmetry). Now we compute the low-temperature limit of the quantities $\bar{R}_v^k$ with $k = 1, 2$. A simple calculation yields, in the limit $T \rightarrow 0$ keeping terms up to first order in T , $\bar{R}_v^1 = 1 - 2T \hat{P}_v(0) + \mathcal{O}(T^2)$, $\bar{R}_v^2 = 1 - \frac{8}{3}T \hat{P}_v(0) + \mathcal{O}(T^2)$. Substituting them into expressions (6), (7), we obtain that both numerator and denominator vanish linearly with T but their ratio remains finite, yielding the expected result,

$$G = \frac{1}{3} + \mathcal{O}(T) \quad (8)$$

$$A = \frac{16T}{3V^4} \sum_{v=1}^V g_v \hat{P}_v(0) v^2 (V - v)^2 + \mathcal{O}(T^2). \quad (9)$$

The only necessary condition to obtain these last results is that $\hat{P}_v(0)$ has a finite weight at zero energy cost for one given volume (v). Otherwise, the expression for $\bar{R}_v^k$ would have corrections of order $\mathcal{O}(T^2)$ and the universal value $1/3$ for G and the linear in T dependence of A would not be recovered anymore [7]. Let us note that in RS we considered one-spin excitations so we assumed that, $\hat{P}_v(0) \neq 0$ for $v = 1$. In that work we stressed that in order to have corrections $\mathcal{O}(T)$ when considering the inversion of two or more spins there had to be singular correlations between local fields at different sites. This is the situation we expect to meet in generic spin glass systems where large cluster excitations are responsible for the universal low-temperature value of G .

4. Scaling theory for OPF fluctuations

Up to now we have only considered the linear terms in a low T expansion. But this first-order term suffices to establish the scaling behaviour of A . In this approach we will focus on large-scale excitations that scale with the volume of the system, assuming that they bring the relevant contribution to thermodynamic quantities. Let us suppose that the weight at zero energy of

lowest excitations scales like $\hat{P}_{v=ld}(0) \sim l^{-\theta'}$, where d is the dimensionality of the system and θ' is the thermal exponent for the lowest excitations. Then we suppose the following scaling ansatz for lowest-lying large-scale excitations:

$$g_v = L^{-\gamma} \hat{g}\left(\frac{v}{L^d}\right) \quad \hat{P}_{v=ld}(0) \sim l^{-\theta'} \quad \frac{v}{V} \propto \mathcal{O}(1) \quad (10)$$

where L is the lattice size and $d \leq \gamma$ (since g_v is positive defined and normalizable). This functional form implies that in order to assure the normalization condition $\sum_v g(v) = 1$, the weight of finite volume excitations is $1 - L^{-\gamma}$. Note that, in principle, since excitations of any size are possible, the average volume of the excitations scales like¹ $\bar{v} \sim L^{2d-\gamma}$. Substituting these relations in A into (9) and taking the large L limit we obtain,

$$A = \frac{16}{3} T L^{-\gamma+d-\theta'} \int_0^1 dx \hat{g}(x) x^{2-\frac{\theta'}{d}} (1 + \mathcal{O}(x)). \quad (11)$$

Assuming that $\hat{g}(x)$ decays fast enough for $x \gg 1$ (e.g. exponentially), the general low T scaling $A \sim T L^{-\theta}$, $\theta \equiv \theta' - d + \gamma$ together with relations (10) provide a way to estimate both² θ' and γ . In this scenario, since A is bounded, $A < 1$, the crossover behaviour of A is then determined by the term $T L^{-\theta}$ that gives a typical length scale $l^* \sim T^{1/\theta}$. In usual domain wall scaling theory [8] we expect that, for $\theta < 0$, there is a relation between the thermal exponent θ that accounts for the scaling of the free energy of the largest excitations³, and the correlation length exponent $\nu = -1/\theta$. Below the lower critical dimension d_l we have $\theta \leq 0$. Above d_l , $\theta \geq 0$ and the low-temperature behaviour of A may decide between the two most controversial spin glass scenarios. In the droplet model [8] $\theta > 0$ and $A \sim T/L^\theta$, while in the RSB scenario $\theta = 0$ yielding a finite A at low T in the $L \rightarrow \infty$ limit. This result corresponds to the case where there is a finite probability density of samples with large-scale excitations of finite energy implying that $\hat{P}_v(\Delta E^*)$ for $v \sim V$ is scale independent. The scaling relation $A \sim T/L^\theta$ can be checked by numerical simulations through measurements of A (preliminary results in two and three dimensions agree with that expression [9, 10]). We note that it holds only for $T/L^\theta \ll 1$ (where the approximation (4) is valid) and does not invalidate the present analysis for $\theta < 0$ if T is low enough.

5. The Ising spin glass chain

An illustrative example of these results is the Ising spin glass chain⁴ which is described by the following Hamiltonian:

$$\mathcal{H} = - \sum_{i=1}^L J_i \sigma_i \sigma_{i+1} \quad (12)$$

where the quenched disorder is distributed according to some continuous distribution $P(J)$ with finite weight at zero coupling. The ground state is unique (up to a global spin inversion) and has an energy $E_{\text{GS}} = - \sum_i J_i \sigma_i^* \sigma_{i+1}^*$. In the study of the low-temperature excitations we have to distinguish between the cases with free and periodic boundary conditions. In the free boundary case the minimum cost excitations correspond to breaking the weakest bond J^* and reversing all the spins on the right or left of that bond. The energy cost of such an

¹ Note that the average volume of the excitations has a lower bound ($\bar{v} \geq 1$), so that this relation holds provided $2d - \gamma \geq 0$.

² A less rigorous derivation of the scaling behaviour for A has also been shown by Drossel *et al* in [4].

³ In principle, θ' may be different from the usual thermal exponent θ in domain wall theory that governs the change in the ground-state energy when modifying the boundary conditions from periodic to antiperiodic or random.

⁴ We are indebted to A J Bray for bringing our attention to this particular example.

excitation reads: $\Delta E^* = 2|J^*|$. Note that depending on the sample, the length of the droplet (v) can range between 1 and $L - 1$. Clearly these excitations have a finite probability of having zero cost as $\hat{P}(\Delta E^* = 0) \sim L P(J^* = 0)$, which is finite by hypothesis. Hence from our previous general arguments it follows that at $T = 0$ we obtain the universal value $G = 1/3$ in agreement with the analytical result derived in RS. It is important to realize that one-spin excitations cannot correspond to minimum cost excitations when considering spins that are not at the boundaries. This is due to the fact that, in this particular system, the ground state is not frustrated. Exciting one interior spin would necessarily frustrate two bonds so that the energy cost would be: $\Delta E^* = 2(|J_i| + |J_k|)$, which is obviously less favourable than breaking a single bond. It is easy to check that $g_v = \frac{1}{L}$ substituted in (9) yields $A = \frac{8P(0)T(L^4-1)}{45L^3}$ in full agreement with transfer matrix calculations shown in RS. Equations (10), (11) with $\gamma = d = 1$ yield $\theta' = -1$.

In the periodic boundary conditions case, the situation is different. Here we have L spins and L couplings, with the condition $\sigma_{L+1} = \sigma_1$. Note that the ground state can have frustrated bonds, so that we can distinguish between two different kinds of samples: non-frustrated (NF) having $\prod_i J_i > 0$ and frustrated (F) having $\prod_i J_i < 0$. In the first case the ground-state energy reads: $E_{\text{NF}}^* = -\sum_i |J_i|$ while in the second we have that the weakest bond, let us say J_k , is unsatisfied so that the ground-state energy reads: $E_{\text{F}}^* = E_{\text{NF}}^* + 2|J_k|$. In both cases, the minimum energy excitation will correspond to breaking the two weakest bonds, let us say (i, k) , but the energy cost will read differently in each case: $\Delta E_{\text{NF}}^* = 2(|J_i| + |J_k|)$, $\Delta E_{\text{F}}^* = 2(|J_i| - |J_k|)$. From here, it is evident that the energy gap in the F set will be much smaller than in the NF set. Thus, only F samples yield contributions $\mathcal{O}(T)$ at low temperatures⁵. In other words, $\hat{P}(\Delta E_{\text{F}}^* = 0) \neq 0$ while $\hat{P}(\Delta E_{\text{NF}}^* = 0) = 0$ although, on average, still $G(T = 0) = 1/3$ and $A \sim TL$.

We conclude with a summary of our results. A low T expansion for OPF reveals that the only condition to obtain $G = 1/3 + \mathcal{O}(T)$ and $A \sim T$ is that the ground state is unique and that the disorder average probability distribution for the lowest excitations is gapless and with finite weight at zero excitation energy. This illustrates the importance of rare samples in determining the low-temperature properties of spin glasses. Assuming that the statistics of the large-scale lowest excitations determines the low T thermodynamic behaviour, usual scaling arguments yield $\hat{P}_{V=L^d}(0) \sim L^{-\theta'}$ and $A \sim TL^{-\theta}$ providing a way to estimate θ' and θ . In this direction, numerical investigation of the first lowest excitations in two-dimensional spin glasses [9, 11] would be welcome to confirm the validity of the scenario we have put forward through the scaling relations (10). Let us also mention that most of the predictions presented here (in particular relations (8), (9), (11)) can be checked with numerical simulations for small sizes thermalized at low temperatures [2]. The calculations shown here open other possibilities. Here we concentrated our attention on the study of the parameter q , which gives information about the size of the excitations. To investigate other topological aspects of the excitations (for instance, their fractal surface exponent d_s), a similar study of OPF for energy or link overlaps along the present lines should be necessary. Further information about the topology of the excitations can be obtained by imposing $G = 1/3$ to all orders in T , a result which apparently holds in spin glasses in the large volume limit.

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⁵ This has been numerically checked by transfer matrix methods. F samples yield $G = 1/3$ at $T = 0$ while NF samples yield a lower value of G at $T = 0$.

References

- [1] Palassini M and Young A P 1999 *Phys. Rev. Lett.* **83** 5126
Palassini M and Young A P 2000 *Phys. Rev. Lett.* **85** 3017
Krzakala F and Martin O C 2000 *Phys. Rev. Lett.* **85** 3013
Marinari E and Parisi G 2001 *Phys. Rev. Lett.* **86** 3887–90
Marinari E and Parisi G 2000 *Phys. Rev. B* **62** 11677
Newman C M and Stein D L 2000 *Preprint* cond-mat/0010033
- [2] Katzgraber H G, Palassini M and Young A P 2000 *Preprint* cond-mat/0007113
Hatano N and Gubernatis J E 2000 *Preprint* cond-mat/0008115
Houdayer J, Krzakala F, Martin O C 2000 *Preprint* cond-mat/0009382
Marinari E, Parisi G, Ricci-Tersenghi F and Zuliani F 2000 *Preprint* cond-mat/0011039
- [3] Marinari E *et al* 1998 *Phys. Rev. Lett.* **81** 1998
Bokil H *et al* 1999 *Phys. Rev. Lett.* **82** 5174
Marinari E *et al* 1999 *Phys. Rev. Lett.* **82** 5175
- [4] Parisi G, Picco M and Ritort F 1999 *Phys. Rev. E* **60** 58
Hukushima K and Kawamura H 2000 *Phys. Rev. E* **62** 3360
Pagnani A, Parisi G and Ricci-Tersenghi F 2000 *Phys. Rev. Lett.* **84** 2026
Ballesteros H G *et al* 2000 *Preprint* cond-mat/0006211
Drossel B, Bokil H and Moore M A 2000 *Phys. Rev. E* **62** 7690
- [5] Picco M, Ritort F and Sales M 2001 *Eur. Phys. J. B* **19** 565–82
- [6] Guerra F 1996 *Int. J. Mod. Phys. B* **10** 1675
- [7] Ritort F and Sales M 2000 *J. Phys. A: Math. Gen.* **33** 6505
- [8] McMillan W L 1984 *J. Phys. C: Solid State Phys.* **17** 3179
Bray A J and Moore M A 1986 *Heidelberg Colloquium on Glassy Dynamics and Optimization* ed L van Hemmen and I Morgenstern (Berlin: Springer)
Fisher D S and Huse D A 1988 *Phys. Rev. B* **38** 386
- [9] Picco M, Ritort F and Sales M 2001 work in progress
- [10] Palassini M unpublished
- [11] Kawashima N 1999 *Preprint* cond-mat/9910366