J. Phys. A: Math. Gen. **33** (2000) 6505–6526. Printed in the UK PII: S0305-4470(00)12828-8

A conjectured scenario for order-parameter fluctuations in spin glasses

Felix Ritort and Marta Sales

Department of Physics, Faculty of Physics, University of Barcelona, Diagonal 647, 08028 Barcelona, Spain

Received 23 March 2000, in final form 14 June 2000

Abstract. We study order-parameter fluctuations (OPF) in disordered systems by considering the behaviour of some recently introduced parameters G, G_c which have proven very useful in locating phase transitions. We prove that both parameters G (for disconnected overlap disorder averages) and G_c (for connected disorder averages) take the respective universal values $\frac{1}{3}$ and $\frac{13}{31}$ in the $T \to 0$ limit for any *finite* volume provided the ground state is *unique* and there is no gap in the ground-state local-field distributions, conditions which are met in generic spin-glass models with continuous couplings and no gap at zero coupling. This makes G, G_c ideal parameters to locate phase transitions in disordered systems much like the Binder cumulant for ordered systems. We check our results by exactly computing OPF in a simple example of uncoupled spins in the presence of random fields and the one-dimensional Ising spin glass. At finite temperatures, we discuss under which conditions the value $\frac{1}{3}$ for G may be recovered by conjecturing different scenarios depending on whether OPF are finite or vanish in the infinite-volume limit. In particular, we discuss replica equivalence and its natural consequence $\lim_{V\to\infty} G(V, T) = \frac{1}{3}$ when OPF are finite. As an example of a model where OPF vanish and replica equivalence does not give information about G we study the Sherrington–Kirkpatrick spherical spin-glass model by performing numerical simulations for small sizes. Again we find results compatible with $G = \frac{1}{3}$ in the spin-glass phase.

1. Introduction

It is well known that mean-field spin glasses are characterized by strong (non-vanishing in the thermodynamic limit) sample-to-sample fluctuations of the order parameter [1]. Despite the fact that extensive thermodynamic quantities (such as free energy and all its finite-order derivatives) are self-averaging in the thermodynamic limit (i.e. their intensive part does not depend on the realization of the quenched randomness) the same result cannot be extended to order parameter fluctuations. It is widely believed that the absence of self-averaging of the order parameter is strongly related to replica symmetry breaking, i.e. the existence of several ergodic components not related by any symmetry of the Hamiltonian.

Recently, Guerra suggested [2] that sample-to-sample fluctuations of the order parameter (hereafter referred to as OPF) verify some sum rules which are generally valid in any disordered system. This claim assumes that the system is stochastically stable in the presence of a mean-field perturbation, a property which may depend strongly on the nature of the equilibrium state. A system is stochastically stable [3] if its properties (static or dynamic) change smoothly in the presence of a small random perturbation. These sum rules have been used recently to define a new dimensionless parameter (hereafter called G) which takes into account sample-to-sample fluctuations [4]. This parameter has been shown to provide an alternative and powerful way of locating phase transition points in disordered systems. The advantage of G with respect to

0305-4470/00/376505+22$30.00

more canonical ones (such as the Binder cumulant ratio used in ordered systems) relies on the fact that it also works very well in the absence of time-reversal symmetry in the Hamiltonian or other more complex disordered systems. In particular, the method has been applied recently for Ising spin glasses [4, 5], Migdal–Kadanoff spin glasses (Bokil *et al* in [4]), Potts glasses [7], Heisenberg spin glasses, which display a chiral phase transition [6] as well as some protein folding models [8].

The purpose of this paper is to show, by using general arguments, analytic computations for simple models and numerical simulations, that indeed this new parameter is an appropriate tool for investigating phase transitions in disordered systems much like the Binder cumulant is for ordered systems. We conjecture and prove that this parameter G takes the universal value $\frac{1}{3}$ at zero temperature for any disordered system (finite or infinite) with the only condition of *uniqueness* of the ground state and the absence of a zero-temperature gap in the local field distribution. This condition is satisfied by all spin-glass models with a continuous distribution of couplings and no gap at zero coupling. At finite temperature G certainly depends on the system size. We claim that due to the property of replica equivalence, for models in which OPF are finite, G converges in the infinite-volume limit to zero if the system is in a paramagnetic phase and to the same zero-temperature value $\frac{1}{3}$ if the system is in the spin-glass phase. When OPF vanish this does not necessarily hold and we discuss under what conditions the universal value $\frac{1}{3}$ may be recovered.

The paper is organized as follows. Section 2 is a reminder of the definition of the G parameter as well as some other useful ones. Section 3 presents a detailed computation on a simple disordered model which serves as an illustrative example of the main results. Section 4 proves the zero-temperature conjecture under some general conditions for any disordered system. Section 5 presents detailed calculations on the one-dimensional Ising spin-glass model using the transfer matrix approach. Section 6 addresses the validity of the conjecture at finite temperature by studying the Sherrington–Kirkpatrick (SK) spherical spin glass, a model where OPF vanish. Finally, we discuss the results and present the conclusions.

2. The G parameter and replica equivalence

The definition of the G parameter is based on some exact relations obtained for the sample-to-sample fluctuations of the order parameter in the Sherrington–Kirkpatrick model [1]. The SK model is defined by the disordered mean-field Hamiltonian

$$\mathcal{H}_{SK} = -\sum_{i<j} J_{ij}\,\sigma_i\,\sigma_j \tag{1}$$

where the J_{ij} are quenched Gaussian variables with zero average and variance $1/N$, where N is the number of sites. The SK model presents a second-order phase transition at $T_c = 1$ below which replica symmetry breaks down and ergodicity is broken. The spin-glass phase is described by an order parameter function $P_J(q_{12})$, where $q_{12} = \sum_{i=1}^{N} \sigma_i^1 \sigma_i^2$ is the replica overlap and the subindex J denotes the realization of the quenched randomness. $P_J(q)$ is a simple object in the paramagnetic phase above T_c ($P_J(q) = \delta(q)$) but develops strong sample-to-sample fluctuations below T_c inside the spin-glass phase. Fluctuations in the order parameter were originally derived by Bray *et al* [10] using the property of replica equivalence [11]. This property states that the sum of all elements contained in a given row (or column) in the replica matrix Q_{ab} is independent of the row (or column). As shown by Parisi [11] this is a necessary condition for the replicated free energy to be proportional to the number of replicas n and have a well defined free energy in the limit $n \to 0$. Fluctuations are then described by

the following exact relation in the $N \to \infty$ limit [9]:

$$\overline{P_J(q_{12}, q_{34})} = \frac{1}{3}\overline{P_J(q_{12})}\delta(q_{12} - q_{34}) + \frac{2}{3}\overline{P_J(q_{12})P_J(q_{34})} \tag{2}$$

where $\overline{(\cdot)}$ denotes a disorder average and 1, 2, 3, 4 denote replica indices. Therefore

$$\overline{P_J(q_{12}, q_{34})} \neq \overline{P_J(q_{12})P_J(q_{34})} \tag{3}$$

so P_J fluctuates with J_{ij} in a non-trivial way. Multiplying both sides of equation (2) by q_{12}^2 and q_{34}^2 and integrating over all possible values of the overlaps q_{12}, q_{34} one obtains the following sum rule [10]:

$$\overline{\langle q_{12}^2 \rangle^2} = \frac{1}{3}\overline{\langle q_{12}^4 \rangle} + \frac{2}{3}\overline{\langle q_{12} \rangle}^2. \tag{4}$$

where $\langle \cdots \rangle$ denotes a thermal average. This relationship has been also rederived by Guerra using general arguments based on self-averaging properties of the internal energy as well as its finite derivatives [2]. Now let us define the following ratio:

$$G = \frac{\overline{\langle q^2 \rangle^2} - \overline{\langle q^2 \rangle}^2}{\overline{\langle q^4 \rangle} - \overline{\langle q^2 \rangle}^2}. \tag{5}$$

Note that the numerator in (5) corresponds (except for the absence of a multiplicative constant N^2) to the sample fluctuations of the spin-glass susceptibility. For the SK model, because of the sum rule (2), it is possible to show that G takes only two values. G is equal to $\frac{1}{3}$ in the replica symmetry broken phase and vanishes above T_c:

$$G = \frac{1}{3}\Theta(T_c - T). \tag{6}$$

The generality of the replica-equivalence property suggests that (6) will hold in any system (even beyond mean-field) if OPF does not vanish in the limit $V \to \infty$. However, it may well happen that OPF vanish. Then both the numerator and the denominator in (5) vanish in the $V \to \infty$ limit. In this case replica equivalence is not enough to decide what the value of G is. The value of G is then determined by the form of the finite-size corrections to the order parameter (and in particular its prefactors), which in principle could not satisfy sum rules such as (4). Despite this uncertainty, in this paper we propose three possible scenarios for the parameter G.

(a) OPF remain finite in the thermodynamic limit. This is the general situation encountered in mean-field models with a replica broken phase. So both the numerator and the denominator in (5) are finite in the infinite-volume limit. The property of replica equivalence and also stochastic stability indicate that the same should be valid for any finite-dimensional disordered system (assuming that for those systems OPF are finite) leading to $G = \frac{1}{3}$ in the spin-glass phase.

(b) OPF vanish in the large-volume limit like $1/V$. This is the situation typically encountered in the paramagnetic phase. The ratio may then be zero or finite depending on the particular case.

(c) OPF vanish in the large-volume limit slower than $1/V$ (for instance, like $1/V^\alpha$ with $\alpha < 1$). This situation is typical of disordered systems with a marginally stable replica symmetric phase. Both the numerator and the denominator in (5) vanish, the ratio G is finite but may be different from $\frac{1}{3}$ at finite temperature. In this case the property of replica equivalence cannot be used for the reason discussed before and stochastic stability may not

hold. Actually the property of stochastic stability may break down if the equilibrium phase is drastically changed in the presence of a mean-field perturbation. This situation may be found in spin-glass models without OPF such as hierarchical lattices (i.e. spin glasses in the Migdal–Kadanoff approximation), the Sherrington–Kirkpatrick spherical spin glass (see section 6) or finite-dimensional models described by a unique low-temperature state such as the droplet model.

Although the main hypothesis of stochastic stability still remains to be proven, all three previous cases seem quite reasonable and we do not know of non-trivial counterexamples. Note that there is no direct relationship between OPF and the value of G in the low-temperature phase. Actually, the previous possibilities (a) and (c) may yield the same value of G, although the physical description of the low-temperature phase is very different. As has been observed by Bokil *et al* in [4], the non-vanishing of G should not be taken as direct evidence for non-vanishing OPF or replica symmetry breaking. In order to make it more evident whether OPF survive in the infinite-volume limit, it is necessary to consider another dimensionless parameter, which does not have the ambiguity of the ratio of two vanishing quantities. For instance, one may define the A parameter [4]

$$A = \frac{\overline{\langle q^2\rangle^2} - \overline{\langle q^2\rangle}^2}{\overline{\langle q^2\rangle}^2} \tag{7}$$

which is nothing other than the numerator of (5) appropriately normalized. We will see later that the nice properties of G are not present in the parameter A and the former is much more convenient for locating phase transitions. Generally, one expects A to be a non-trivial function of both volume and temperature vanishing (in the $V \to \infty$ limit) only when OPF vanish (for instance, in a paramagnetic phase). If OPF are finite A may take a finite value but an identity such as (6) for A does not hold.

In this paper we will show examples for all three behaviours, by explicit analytic computations and some numerical calculations. Furthermore, we will show that, for models with a unique ground state and without a gap in the ground-state local field distribution,

$$\lim_{T\to 0} G(V,T) = \frac{1}{3} \tag{8}$$

so the G parameter is $\frac{1}{3}$ at $T = 0$ for *any* finite volume V. This is no longer true at finite temperature where the parameter G may take the value $\frac{1}{3}$ only in the infinite-volume limit.

Before finishing this section let us remind the reader that in [4, 5] other quantities similar to (5) and (7) have been proposed for systems without time-reversal symmetry. These are defined by considering the *connected* overlaps

$$G_c = \frac{\overline{\langle (q-\langle q\rangle)^2\rangle^2} - \overline{\langle (q-\langle q\rangle)^2\rangle}^2}{\overline{\langle (q-\langle q\rangle)^4\rangle} - \overline{\langle (q-\langle q\rangle)^2\rangle}^2} \tag{9}$$

$$A_c = \frac{\overline{\langle (q-\langle q\rangle)^2\rangle^2} - \overline{\langle (q-\langle q\rangle)^2\rangle}^2}{\overline{\langle (q-\langle q\rangle)^2\rangle}^2}. \tag{10}$$

We will see that a result like (8) also applies to the parameter G_c and our result reads

$$\lim_{T\to 0} G_c(V,T) = \frac{13}{31}. \tag{11}$$

For the SK model the quantity G_c is defined by restricting thermal averages to the $q > 0$ part of $P(q)$. G_c does not satisfy the identity (6) so this is not the best quantity to look at

in numerical simulations, despite the fact that both G_c and G (and also A_c and A) may take similar values in the vicinity of the critical region. This explains why similar results were obtained for both sets of quantities in numerical simulations.

3. An instructive example

Here we analyse in detail a solvable case which will be useful to illustrate the main contents of the paper and how disorder expectation values of the overlaps are computed. Moreover, the analysis of this section will prove to be useful for a constructive proof of the zero-temperature results (8) and (11) to be presented later on. Consider the following Hamiltonian:

$$\mathcal{H} = -\sum_{i=1}^{V} h_i \sigma_i \tag{12}$$

where the spins may take the values ± 1 and the fields h_i are uncorrelated and randomly taken from a distribution $P(h)$ with finite weight at zero field (i.e. $P(0)$ finite). In principle, $P(h)$ may be any function

$$P(h) = \tilde{P}(h) + \sum_k c_k \delta(h - h_k) \tag{13}$$

with $\tilde{P}(h)$ any continuous function, all $h_k \neq 0$ and $\tilde{P}(0) \neq 0$. This condition is enough to ensure the non-degeneracy of the ground state because there is a single configuration which minimizes the energy $\sigma_i^* = \mathrm{sign}(h_i)$. Note that if a finite fraction of the fields h_i were zero then the ground state would be degenerate. With this very general condition we may exactly compute the parameters G and A introduced in the previous section. Everything reduces to computing the three overlap quantities: $\overline{\langle q^2 \rangle}$, $\overline{\langle q^4 \rangle}$ and $\overline{\langle q^2 \rangle^2}$. The computations are quite elementary and here we present the final results. For the numerator and denominator of equation (5) we obtain

$$\textit{numerator} \equiv \frac{2(V-1)}{V^3}\overline{R^2}^2 + \frac{4(V-1)(V-2)}{V^3}\overline{R^2}\,\overline{R}^2 - \frac{2(2V^2-5V+3)}{V^3}\overline{R}^4 \tag{14}$$

$$\textit{denominator} \equiv \frac{2}{V^2} - \frac{2}{V^3} + \frac{4(V-1)(V-2)}{V^3}\overline{R}^2 - \frac{2(2V^2-5V+3)}{V^3}\overline{R}^4 \tag{15}$$

where

$$\overline{R} = \int_{-\infty}^{\infty} \mathrm{d}h\, P(h) \tanh^2(\beta h) \tag{16}$$

$$\overline{R^2} = \int_{-\infty}^{\infty} \mathrm{d}h\, P(h) \tanh^4(\beta h) \tag{17}$$

and $P(h)$ is the generic distribution (13). The expressions for the parameters G and A may be further simplified, yielding

$$G = \frac{(\overline{R^2} - \overline{R}^2)(\overline{R^2} + (2V-3)\overline{R}^2)}{(1-\overline{R}^2)(1+(2V-3)\overline{R}^2)} \tag{18}$$

and

$$A = \frac{2(V-1)(\overline{R^2} - \overline{R}^2)(\overline{R^2} + (2V-3)\overline{R}^2)}{V(1+(V-1)\overline{R}^2)^2}. \tag{19}$$

Note that in the limit $V \to \infty$ both the numerator and the denominators in (14) and (15) vanish. The quantity A also vanishes like $1/V$ but the ratio G stays finite:

$$\lim_{V\to\infty} G(V,T) = \frac{\overline{R^2} - \overline{R}^2}{1 - \overline{R}^2}. \tag{20}$$

The finite volume quantity $G(T,V)$ in (18) satisfies the conjecture (8). A simple integration by parts reveals that the asymptotic low-temperature behaviour of $\overline{R}$ and $\overline{R^2}$ is given by

$$\overline{R} = 1 - TD + \mathrm{O}(T^2) \qquad \overline{R^2} = \overline{R} - \frac{T}{3}D + \mathrm{O}(T^2) \tag{21}$$

where D is a positive constant given by

$$D = 2P(0). \tag{22}$$

Substituting the asymptotic behaviour (21) in (18) we obtain $G(V, T=0) = \frac{1}{3}$. Note that the same result is obtained by substituting (21) in (20), because in this simple example the two limits $T \to 0$ and $V \to \infty$ may be interchanged. This is not generally true: in particular, when a phase transition takes place at $T = 0$ the two limits may no longer be interchanged.

For the parameters G_c and A_c introduced in (9) and (10) we obtain

$$G_c = \frac{\overline{R^4} - (\overline{R^2})^2}{2V - 2 - 4(V-2)\overline{R^2} + (2V-3)(\overline{R^2})^2 - 3\overline{R^4}} \tag{23}$$

$$A_c = \frac{\overline{R^4} - (\overline{R^2})^2}{V(1-\overline{R^2})^2}. \tag{24}$$

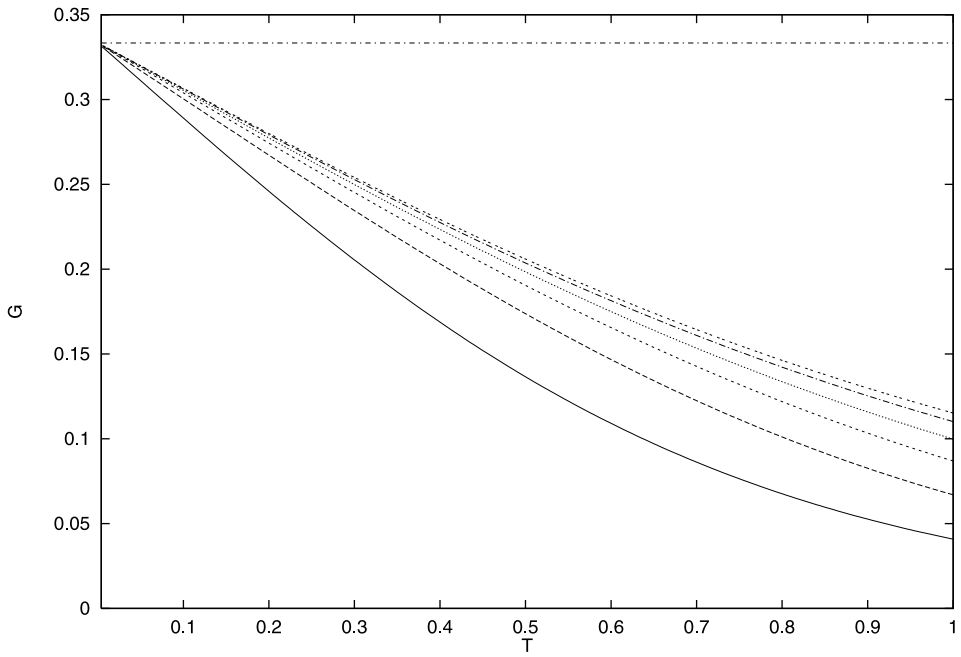

Figure 1. Parameter G for $V = 2, 4, 8, 16, 50, 100$ from top to bottom.

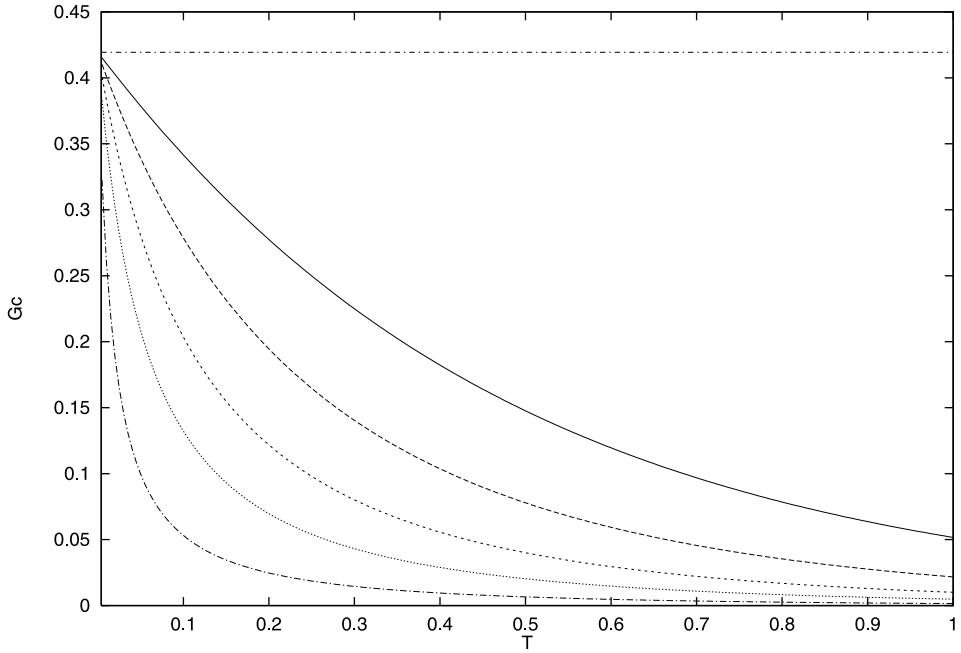

Figure 2. Parameter G_c for $V = 2, 4, 8, 16, 50$ from top to bottom.

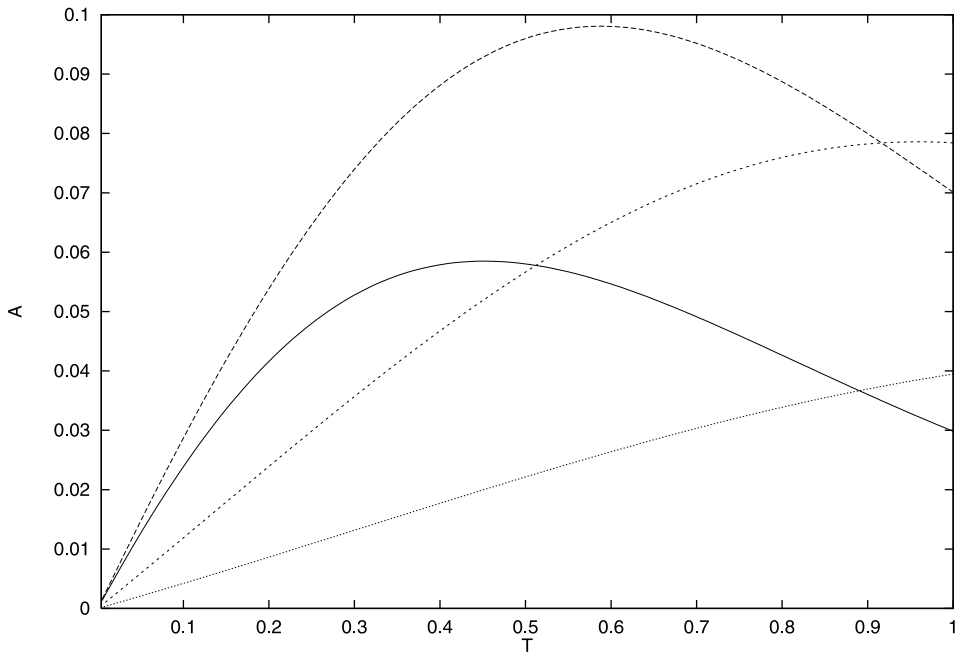

Figure 3. Parameter A for $V = 2, 4, 8, 16, 50$ from top to bottom.

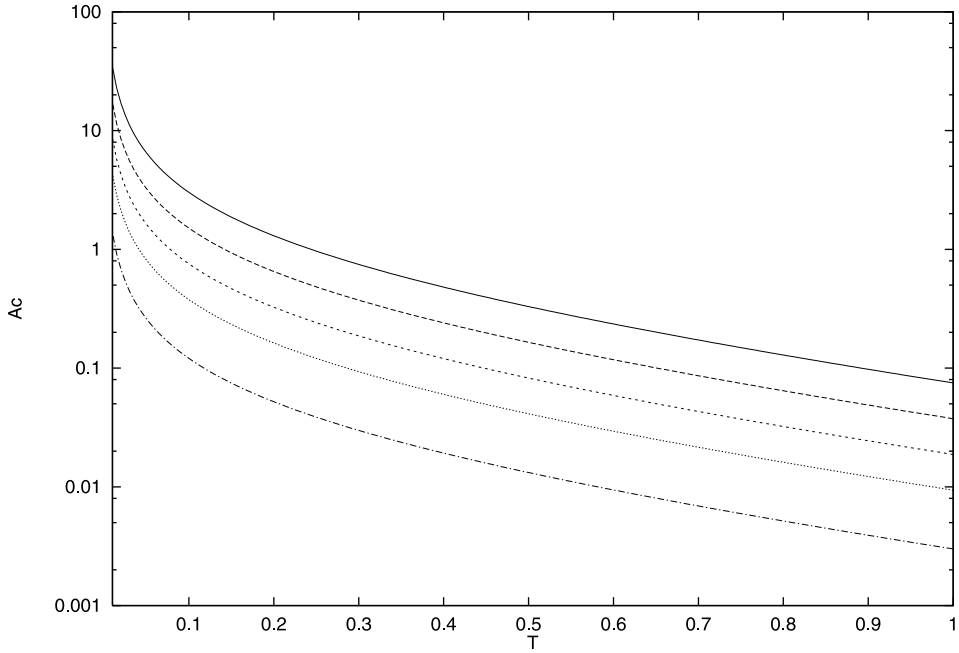

Figure 4. Parameter A_c for $V = 2$ (full), 4 (long-broken), 16 (short-broken), 50 (dotted).

We observe that G_c behaves in a different way. It tends to zero for T finite and is again independent of the volume for $T = 0$ but takes the value $\frac{13}{31}$. For G_c the two limits ($V \to \infty$ and $T \to 0$) now do not commute. Figures 1–4 show the behaviour of G, G_c, A, A_c as functions of temperature for different values of V for the case of a Gaussian fields distribution $P(h) = (2\Pi)^{-1/2} \exp(-h^2/2)$.

In the case of a gap of amplitude Δ in the field distribution one finds that both A and G vanish exponentially with that gap $G \sim T \exp(-\beta\Delta)$ and the conjecture no longer holds.

We will now prove that, under some general conditions, the conjectured zero-temperature values for G and G_c hold for any disordered system.

4. A proof of the conjecture

To generally prove (8) and (11) we start by considering a general Hamiltonian $\mathcal{H}(\{\sigma\})$ where the $\{\sigma_i; i = 1, \ldots, V\}$ are Ising variables which may take the values ± 1†. This Hamiltonian may be written in terms of the local fields

$$\mathcal{H} = -\sum_{i=1}^{V} h_i \sigma_i \tag{25}$$

where the h_i are local fields proportional to

$$h_i \propto \frac{\partial \mathcal{H}}{\partial \sigma_i} \tag{26}$$

† The present demonstration holds for models described by discrete variables. For continuous models the considerations may completely change because the nature of the low-temperature excitations is different.

which depend on the configuration $\{\sigma\}$. Suppose now that the Hamiltonian $\mathcal{H}$ may only take continuous values so there is no ground-state degeneracy (apart from a global symmetry in the Hamiltonian such as time-reversal symmetry; this case will be discussed below). In particular, no local field h_i vanishes. Let us denote by $\{\sigma^*\}$ the (unique) ground-state configuration. The ground state is stable with respect to all possible numbers of spin flips, so that the value of the energy in that configuration $\mathcal{H}(\{\sigma^*\})$ is an absolute minimum. In particular, the ground state is stable with respect to single spin flips and the local fields evaluated at the ground state satisfy the property

$$\sigma_i^* = \mathrm{sign}(h_i^*) \tag{27}$$

where h_i^* are evaluated at σ^*. To prove the conjecture we need to prove the following statement:

Statement. *Excitations which involve the reversal of a single spin yield the dominant contribution to the low-temperature behaviour for all the quantities* $\overline{(q^k)}^l$ *for any positive integers* k, l *and by extension, to the numerator and denominator in (5), (7), (9) and (10).*

This statement somehow allows us to map the most probable excitations in (25) with those of the instructive example presented before (12). Nevertheless, we must emphasize two points. The first one is that the ground-state local field distribution in the previous example (12) was taken as uncorrelated for different sites and also the same distribution was taken for each spin i. In general, this is not true. Local fields at different sites may be correlated and the distribution on a given site may depend on the site. For instance, in models with open boundaries the local field distribution for the sites located on the surface is certainly different from the distribution of those in the bulk. The second observation is that, in general, the lowest excitations in (25) may involve groups of several spins (and not a single spin flip like in the simple case (12)). So in order to prove the conjecture we must show that excitations in (25) which involve the reversal of any number of spins larger than one always yield sub-dominant low-temperature corrections to the single-spin excitation case.

In what follows we present a constructive proof of the previous statement without the need to refer to the results of the instructive example which had some restrictive assumptions. We start from the general Hamiltonian (25) and analyse the low-temperature behaviour of the order parameters $\overline{\langle q^2\rangle}$, $\overline{\langle q^4\rangle}$ and $\overline{\langle q^2\rangle^2}$. We will first consider the case of one spin excitations and later on the more general one of higher-order excitations.

One-spin excitations

The calculation proceeds as follows. Consider the ground state $\{\sigma^*\}$ of (25) as *unique* and one-spin excitations which involve the reversal of a single spin. If we consider the ground state plus this class of V possible excitations we can compute the correlation function $\langle\sigma_i\sigma_j\rangle$ $(i \neq j)$, obtaining the result

$$\langle\sigma_i\sigma_j\rangle = \sigma_i^*\sigma_j^*\left(1 - 2\frac{\exp(-2\beta h_i^*\sigma_i^*) + \exp(-2\beta h_j^*\sigma_j^*)}{1 + \sum_{l=1}^{V}\exp(-2\beta h_l^*\sigma_l^*)}\right). \tag{28}$$

In the low-T limit, provided $TV \ll 1$, we will see that this expression coincides with that obtained by expanding $\langle\sigma_i\sigma_j\rangle$ around its ground-state value $\sigma_i^*\sigma_j^*$, as including higher-order excitations yields sub-dominant corrections to the correlation function. Defining $x_i = \exp(-2\beta h_i^*\sigma_i^*)$, we find in the $\beta \to \infty$ limit

$$\langle\sigma_i\sigma_j\rangle = \sigma_i^*\sigma_j^*(1 - 2(x_i + x_j)) \qquad (i \neq j) \tag{29}$$

where we have approximated by 1 the term in the denominator of the ratio in (28). Such an approximation is allowed provided one performs the limit $\beta \to \infty$ *before* the infinite-volume limit. Note that, in that denominator, each exponential contributes to the sum at most with a term proportional to the temperature (see below). Because there are V terms of that type, at most that term is of order VT. Hence, in the limit $TV \ll 1$, that denominator equals 1. The result (29) is the only quantity we need in order to evaluate $\langle q^2 \rangle$ and $\langle q^2 \rangle^2$. In terms of the variable $T_{ij} = \langle \sigma_i \sigma_j \rangle^2$, these are given by

$$\langle q^2 \rangle = \frac{1}{V} + \frac{1}{V^2} \sum_{i \neq j} T_{ij} \tag{30}$$

$$\langle q^2 \rangle^2 = \frac{1}{V^2} + \frac{2}{V^3} \sum_{i \neq j} T_{ij} + \frac{2}{V^4} \sum_{i \neq j} T_{ij}^2 + \frac{4}{V^4} \sum_{(i \neq j \neq k)} T_{ij} T_{ik} + \frac{1}{V^4} \sum_{(i \neq j \neq k \neq l)} T_{ij} T_{kl} \tag{31}$$

where the indices in the sums run from 1 to V and correspond to different sites. To average (30) and (31) over the disorder we need to compute disorder averages of terms of the type $x_i^m x_j^n$, where i, j denote sites and m, n positive integers. It is easy to show that, in the absence of a gap in the ground-state local-field distribution, the terms with $i = j$ yield the dominant low-temperature corrections and vanish linearly with T. Terms with $i \neq j$ yield higher-order $\mathrm{O}(T^2)$ contributions. Suppose $P(\{h_i^*\})$ denotes the ground-state local-field probability distribution. For the terms $x_i^m x_j^n$ $(i \neq j)$, we have

$$\overline{x_i^m x_j^n} = \int_{-\infty}^{\infty} \exp(-2m\beta h_i^* \sigma_i^*) \exp(-2n\beta h_j^* \sigma_j^*) P(h_1^*, \ldots, h_V^*) \, \mathrm{d}h_1^* \ldots \mathrm{d}h_V^*. \tag{32}$$

The field variables h_k^* $(k \neq i, j)$ may be integrated out, yielding the following expression:

$$\overline{x_i^m x_j^n} = \int_{-\infty}^{\infty} \exp(-2m\beta h_i^* \sigma_i^*) \exp(-2n\beta h_j^* \sigma_j^*) \, \hat{P}_{ij}(h_i^*, h_j^*) \, \mathrm{d}h_i^* \, \mathrm{d}h_j^* \tag{33}$$

$$\hat{P}_{ij}(h_i^*, h_j^*) = \int_{-\infty}^{\infty} P(h_1^*, \ldots, h_V^*) \prod_{k \neq (i,j)} \mathrm{d}h_k^*. \tag{34}$$

If the local field distribution $P(\{h_i^*\})$ has finite weight at the point $h_i = 0 \, \forall i$, then the same holds for the two-sites probability $\hat{P}_{ij}(0, 0)$, so that we may expand this term around $(0, 0)$ in (33), thereby obtaining

$$\overline{x_i^m x_j^n} = \int_{-\infty}^{\infty} \exp(-2m\beta h_i^* \sigma_i^*) \exp(-2n\beta h_j^* \sigma_j^*) \times \left(\hat{P}_{ij}(0, 0) + \left(\frac{\partial \hat{P}_{ij}}{\partial h_i^*} \right)_{(0,0)} h_i^* + \left(\frac{\partial \hat{P}_{ij}}{\partial h_j^*} \right)_{(0,0)} h_j^* + \mathrm{O}(h_i^* h_j^*) \right) \mathrm{d}h_i^* \, \mathrm{d}h_j^* \tag{35}$$

where $\mathrm{O}(h_i^* h_j^*)$ denotes higher-order terms at least quadratic in the fields. On writing equation (35) our main assumption comes from the fact that, as we are dealing with a finite system $\hat{P}(h_i^*, h_j^*)$ has no singular contributions (i.e. there are no contributions of the type $\delta(h_i^* - h_j^*)$). Therefore, $\hat{P}(h_i^*, h_j^*)$ is finite and analytic at any point and, in particular, at $(0, 0)$ so that it can be Taylor expanded around that point. All the same, our assumptions are a direct consequence of the fact that only in the thermodynamic limit do we expect to find singular correlations between fields at different sites. A simple saddle-point calculation (in the $\beta \to \infty$ limit) then gives

$$\overline{x_i^m x_j^n} = \frac{T^2}{mn} \hat{P}_{ij}(0, 0) + \mathrm{O}(T^3). \tag{36}$$

The dominant terms in the limit $T \to 0$ correspond to terms of the type $\overline{x_i^n}$, which give

$$\overline{x_i^n} = \frac{T\hat{P}_i(0)}{n} \tag{37}$$

where $\hat{P}_i(0)$ is the value of the single-site probability distribution on the site i evaluated at $h = 0$:

$$\hat{P}_i(h^*) = \int_{-\infty}^{\infty} P(h_1, \ldots, h_V)\delta(h_i - h^*) \prod_{k \neq i} \mathrm{d}h_k. \tag{38}$$

This probability is not independent of the spin i, as our Hamiltonian can contain terms which introduce asymmetry between different sites. This is an important difference with respect to the computation of the previous section where the local field distribution (13) was site independent. Actually, this independence was necessary in the 'instructive example' to fully carry out the analytic computation of G and G_c. The key point is that, at the level of one-spin excitations, low-temperature corrections to overlap averages are linear in T and $\hat{P}_i(0)$. According to expressions (30) and (31) all sites are equivalent (inequivalence of sites enters only through the value of $\hat{P}_i(0)$), so the only invariant term linear in P is $\sum_i \hat{P}_i(0)$. The numerator in (5) yields

$$\overline{\langle q^2\rangle^2} - \overline{\langle q^2\rangle}^2 = \frac{16T\sum_i P_i(0)}{3V^4}(V-1)^2 + \mathrm{O}(T^2). \tag{39}$$

To compute the overlap $\overline{\langle q^4\rangle}$ we use the expression

$$\overline{\langle q^4\rangle} = \frac{1}{V^4}\left(3V^2 - 2V + (6V-8)\sum_{i\neq j} T_{ij} + \sum_{(i,j,k,l)} T_{ijkl}\right) \tag{40}$$

where $T_{ijkl} = \langle \sigma_i\sigma_j\sigma_k\sigma_l\rangle^2$. Similarly, as for the two-point correlation function (29) we obtain

$$\langle \sigma_i\sigma_j\sigma_k\sigma_l\rangle = \sigma_i^*\sigma_j^*\sigma_k^*\sigma_l^*(1 - 2(x_i + x_j + x_k + x_l)) \qquad (i, j, k, l \text{ all different}). \tag{41}$$

With the same assumptions as for the two-point function we obtain for the denominator in (4)

$$\overline{\langle q^4\rangle} - \overline{\langle q^2\rangle}^2 = \frac{16T\sum_i P_i(0)}{V^4}(V-1)^2 + \mathrm{O}(T^2) \tag{42}$$

which finally yields

$$G = \frac{1}{3} + \mathrm{O}(T). \tag{43}$$

A similar calculation for G_c yields $G_c = \frac{13}{31} + \mathrm{O}(T)$.

Two-spin excitations

Let us now consider excitations which involve only two different spins in the lattice ($V(V-1)/2$ different types of excitations). In this calculation one-spin excitations are not included. It is easy to check that these excitations yield $\mathrm{O}(T^2)$ corrections to the two-spin and four-spin correlations. Under the same conditions as before these are given by

$$\langle \sigma_i\sigma_j\rangle = \sigma_i^*\sigma_j^* \frac{(1 + \sum_{k\neq l}(1 - 2\delta_{ki} - 2\delta_{kj} - 2\delta_{li} - 2\delta_{lj})\exp(-2\beta h_k^*\sigma_k^* - 2\beta h_l^*\sigma_l^*))}{1 + \sum_{k\neq l}\exp(-2\beta h_k^*\sigma_k^* - 2\beta h_l^*\sigma_l^*)}$$

$$\overset{\beta V \ll 1}{\approx} \sigma_i^*\sigma_j^*\left(1 - 4(x_i + x_j)\sum_{l\neq i,j} x_l\right) \qquad (i \neq j) \tag{44}$$

$$\langle\sigma_i\sigma_j\sigma_k\sigma_l\rangle = \sigma_i^*\sigma_j^*\sigma_k^*\sigma_l^*\left(1 - 4(x_i + x_j + x_k + x_l)\sum_{m\neq i,j,k,l} x_m\right) \qquad (i, j, k, l \text{ all different}). \tag{45}$$

It could seem that in the expressions above we have dropped the term which accounts for the change in h_i^* due to the flip of σ_j^*, this is, our change in energy should read $\Delta E = 2h_k^*\sigma_k^* + 2h_l^*\sigma_l^* - J_{kl}\sigma_k^*\sigma_k^*$, however, by making the following change: $h_k' = h_k^* - J_{kl}^*\sigma_l^*/2$ we can rewrite ΔE, and thus express the correlation functions in terms of $x_i' = \exp(-2\beta h_i'\sigma_i^*)$. By this change our results should not be altered provided the probability distribution of the h_i' has the same properties as $P(h_i^*, \ldots)$, which is reasonable as we had already considered non-vanishing correlations between fields at different sites. Thus, as we said in the previous discussion after equation (35), in terms such as $\overline{x_i x_j}$ there are no contributions linear in T.

A saddle-point calculation shows that corrections to the ground-state correlation functions are quadratic in T. Finite-T corrections now depend on both $\overline{x_i}\,\overline{x_j}$ and $\overline{x_i x_j}$ for $i \neq j$. Now, for the quantity G we expect a dependence of both numerator and denominator on terms of the type $\hat{P}_i(0)\hat{P}_j(0)$ as well as $\hat{P}_{ij}(0, 0)$. They can enter in different forms, for instance $\sum_{i\neq j}\hat{P}_{ij}(0, 0)$, $\left(\sum_i \hat{P}_i(0)\right)^2$ or $\left(\sum_i \hat{P}_i(0)^2\right)$. A universal value for G is no longer guaranteed. In particular, supposing uncorrelated local fields (which, in principle, may not be true) and independence of the one-site probability distribution $\hat{P}_i(0)$ on the site i we obtain, after a simple but lengthy calculation,

$$\overline{\langle q^2\rangle}^2 - \overline{\langle q^2\rangle}^2 = \frac{128T^2P(0)^2}{9V^3}(V-2)^2(V-1) + \mathrm{O}(T^3) \tag{46}$$

$$\overline{\langle q^4\rangle} - \overline{\langle q^2\rangle}^2 = \frac{64T^2P(0)^2}{V^3}(V-2)^2(V-1) + \mathrm{O}(T^3) \tag{47}$$

and their ratio yields $G = \frac{2}{9} + \mathrm{O}(T)$ which is different from before. We stress again that the result $\frac{2}{9}$ is not universal and will certainly not hold in the most general case. This calculation has been shown to stress how the $\frac{1}{3}$ value is a fingerprint of the dominance in the limit $T \to 0$ of the one-spin excitations.

Higher-order excitations

The generalization to the most general case of K-spin excitations is straightforward. Including only this class of excitations we obtain $\mathrm{O}(T^K)$ corrections to correlations which involve any finite number of spins. This can be easily seen from the fact that any possible excitation of this type will involve the reversal of K different spins, each spin i contributing by a factor $x_i = \exp(-2\beta h_i^*)$ to the correction. The simultaneous effect of all spins yields a product type $\prod_{i=1}^K x_i$ which immediately gives (in the limit $\beta \to \infty$) the T^K term. The numerator and denominator in G are of order T^K with $\mathrm{O}(T^{K+1})$ corrections. The final result for G for any value of K is not easy to compute and, as previously discussed, will depend on a larger number of invariants, which involve different combinations of the terms $\hat{P}_i(0), \hat{P}_{i_1 i_2}(0, 0), \ldots, \hat{P}_{i_1,\ldots,i_K}(0, 0)$.

When all possible excitations are treated together the calculation proceeds as before. The dominant contribution for OPF will always come from samples whose lowest excitations are one-spin excitations. Consequently, in the zero-temperature limit (for V finite) one-spin excitations dominate the correction to correlation functions, proving our conjecture. Note that the result we are stating here is quite natural. OPF at very low temperatures are always

dominated by those rare samples characterized by local fields $\beta h \ll 1$ where one-spin-excitations yield the largest contribution. From a numerical point of view this implies that more samples are needed to compute the values of G and G_c with a reasonable precision as T goes down. This is because for $T \to 0$ the effect from rare samples on OPF becomes more and more important. Let us stress again that the present derivation assumed that $TV \ll 1$. In the opposite limit or in an intermediate regime the result obviously does not hold. In that case, it may well happen that dominant contributions in OPF involve the reversal of a large number of spins (domain excitations) which, in the limit $TV \gg 1$, may also involve the whole system [19].

The hypothesis of a unique ground state is apparently in contradiction with the case in which there is time-reversal symmetry. Indeed, all spin correlations computed in this section are invariant under time-reversal symmetry and the present conclusions remain unchanged. The situation is certainly different in disordered systems with non-trivially degenerate ground states (for instance, finite-dimensional spin glasses with discrete couplings) where we expect that $G(V, T)$ vanishes exponentially with $1/T$ like in the instructive example of the previous section. Again, in the other limit (finite temperature and $V \to \infty$) the behaviour of these degenerate models may completely change and G could be finite again†.

5. The 1D Ising spin glass

In this section we present an analysis of the one-dimensional (1D) Ising spin-glass model with free boundary conditions. We consider the following Hamiltonian:

$$\mathcal{H} = -\sum_{i=1}^{V-1} J_i \sigma_i \sigma_{i+1} \tag{48}$$

where the couplings are randomly distributed according to the probability distribution $P(J)$. Our aim is to obtain an analytic expression for G and A equations (5) and (7). As this model has the transition at $T = 0$, we expect that in the large-volume limit G will go to zero except at $T = 0$, where $G = \frac{1}{3}$. Moreover, we show that at zero temperature $G = \frac{1}{3}$ for any finite system, although here the two limits ($V \to \infty$ and $T \to 0$) do not commute. In order to obtain an expression for the moment of the order parameter q we have computed the following object:

$$\overline{\langle \mathrm{e}^{yq} \rangle^m} \tag{49}$$

where m is a positive integer and q is the overlap between two different configurations of spins, which is the generator of the moments of the overlap $\overline{\langle q^p \rangle^s}$. Once obtained this expression, by partial derivation respect to y we will obtain expressions for the expectation values of all the moments of q, such as

$$\overline{\langle q^n \rangle} = \left. \frac{\partial^n \overline{\langle \mathrm{e}^{yq} \rangle}}{\partial y^n} \right|_{y=0}. \tag{50}$$

In our computation we are only interested in the quantities $\overline{\langle q^2 \rangle}$, $\overline{\langle q^4 \rangle}$ and $\overline{\langle q^2 \rangle^2}$. Consequently, we only need to compute (49) for $m = 1, 2$. The former can be easily computed by (50). By

† This problem of commutation of limits also appears in the controversy as to whether there are more than two states in finite-dimensional spin glasses. Obviously, there are many ground states in a finite-dimensional spin glass with discrete couplings. The important question is whether many states survive at finite temperatures.

doing some more work we can obtain an expression for $\overline{\langle q^2\rangle^2}$:

$$\overline{\langle q^2\rangle^2} = \frac{1}{3}\left[\frac{\partial^4 \overline{\langle e^{yq}\rangle}^2}{\partial y^4} - \frac{\partial^4 \overline{\langle e^{yq}\rangle}}{\partial y^4}\right]_{y=0} \tag{51}$$

where we have used the fact that in this model $\langle q\rangle = 0$.

5.1. The transfer matrix method

For general m, equation (49) can be computed through the transference matrix method [12]. We have to compute

$$\prod_{\alpha=1}^{m} \frac{\sum_{\{\sigma^\alpha\}\{\tau^\alpha\}} \exp\left(y\sum_{i=1,V}(\sigma_i^\alpha\tau_i^\alpha/V) + \beta\sum_{i=1}^{V-1} J_i(\,\sigma_i^\alpha\sigma_{i+1}^\alpha + \tau_i^\alpha\tau_{i+1}^\alpha)\right)}{\mathcal{Z}^2} \tag{52}$$

where $\mathcal{Z} = 2\prod_i 2\cosh(\beta J_i)$ is the partition function of a 1D chain, α is the index for each pair of replicas and we have m systems of two replicas.

In order to perform the average over the disorder, we are interested in considering the transfer matrix associated with each point i, so that it contains all the dependence of the J_i. For a single pair of replicas this matrix reads

$$V_i \equiv V(\sigma_i, \tau_i; \sigma_{i+1}, \tau_{i+1}) = \frac{\exp\left(y[(\sigma_i\tau_i + \sigma_{i+1}\tau_{i+1})/2N] + \beta J_i(\,\sigma_i\sigma_{i+1} + \tau_i\tau_{i+1})\right)}{(2\cosh(\beta J_i))^2}. \tag{53}$$

For general m our matrix associated with each point consists of the tensorial product of m matrices V_i. At this stage we are ready to perform the average over the disorder and for any i we have

$$\overline{T} = \overline{T_i} = \overline{\bigotimes_1^m V_i}. \tag{54}$$

Then our calculation is reduced to

$$\overline{\langle e^{yq}\rangle^m} = \frac{1}{4}\sum \exp\left[y\frac{\sum_\alpha \sigma_1^\alpha\tau_1^\alpha}{2V}\right]\overline{T}^{V-1}\exp\left[y\frac{\sum_\alpha \sigma_V^\alpha\tau_V^\alpha}{2V}\right] \tag{55}$$

so we must compute the trace of the product

$$\overline{T}^{V-1}B \tag{56}$$

where A is a $4m\times 4m$ matrix, which is the tensorial product of m matrices, which contain the terms of the two edges which had fallen out in the symmetrization process,

$$B = \bigotimes_\alpha \frac{1}{2^2}\exp\left[y\frac{\sigma_1^\alpha\tau_1^\alpha + \sigma_V^\alpha\tau_V^\alpha}{2V}\right]. \tag{57}$$

The rest of the calculation is straightforward. In the first place we have to diagonalize $\overline{T}$, and obtain the set of eigenvalues and eigenvectors, so that in this new base we have

$$\overline{T}_\lambda{}^{V-1} = \begin{pmatrix} \lambda_1^{V-1} & \cdots & \cdots \\ \cdots & \lambda_2^{V-1} & \cdots \\ \cdots & \cdots & \cdots \\ \cdots & \cdots & \lambda_{2^{2m}}^{V-1} \end{pmatrix} \tag{58}$$

where the subindex λ denotes the diagonalized matrix. We then have to obtain the change of base matrix M which expresses the new set of eigenvectors $\{\lambda^i\}$ in terms of the old base $\{\sigma^\alpha\}$. We finally obtain

$$\overline{\langle \mathrm{e}^{yq}\rangle^m} = \mathrm{Tr}\, M\overline{T}_\lambda{}^{V-1} M^T B. \tag{59}$$

We have to point out that the case $m = 1$ is easy to solve. However, the case $m = 2$ turns out to be more difficult as the diagonalization of $\overline{V}$ is not trivial. To compute $\overline{\langle q^2\rangle^2}$ one can always use the traditional method by using the fact that

$$\langle \sigma_i \sigma_j \rangle = \prod_{p=i,\,j-1} \tanh \beta J_p \qquad i \neq j. \tag{60}$$

5.2. Results

Here we report on the results obtained in the low-temperature limit and in the infinite-volume limit. The relevant quantities $\overline{\langle q^2\rangle}$, $\overline{\langle q^4\rangle}$ and $\overline{\langle q^2\rangle^2}$ only depend on V, $\overline{R}$ and $\overline{R^2}$, which have been introduced in section 3, and whose low-temperature behaviour is given by (21). At finite temperature, where $\overline{R}^V$ and $\overline{R^2}^V \ll 1$ we obtain for the numerator and denominator in (5):

$$\textit{numerator} = \frac{4(1+\overline{R})(\overline{R}^2 - \overline{R^2})}{V^3(\overline{R}-1)^3(\overline{R^2}-1)} + \mathcal{O}\left(\frac{1}{V^4}\right) \tag{61}$$

$$\textit{denominator} = \frac{2(1+\overline{R})^2)}{V^2(1-\overline{R})^2} + \mathcal{O}\left(\frac{1}{V^3}\right) \tag{62}$$

where we have kept the lowest orders in $1/V$ and we have made the following approximations $\lim_{V\to\infty} \overline{R}^V$, $\overline{R^2}^V \to 0$. We see that in this limit G goes to zero as $1/V$. However, if we take the low-temperature limit (21), where $\overline{A}$, $\overline{A^2} \approx 1$ then we obtain the expressions

$$\textit{numerator} = \frac{4D(V^4-1)T}{45V^3} + \mathcal{O}(T^2) \tag{63}$$

$$\textit{denominator} = \frac{4D(V^4-1)T}{15V^3} + \mathcal{O}(T^2) \tag{64}$$

where D is given by $D = 2P(0)$. This yields $G = \frac{1}{3} + \mathcal{O}(T)$, independently of the size of the system. A detailed computation up to second order in T gives us that in the large-volume limit: $G = \frac{1}{3} - BTV$, with B being a constant. In fact, for the parameter A, we find in the limit $T \to 0$:

$$A = \frac{4D(V^4-1)T}{45V^3} + \mathcal{O}(T^2). \tag{65}$$

In figures 5 and 6 we show G and A as a function of the temperature for a Gaussian distribution of couplings $P(J) = (2\Pi)^{-1/2}\exp(-J^2/2)$. Note that the low-temperature corrections to G and (65) scale as TV when $V \to \infty$, reflecting the fact that as we get close to the transition point $T = 0$, the correlation length diverges as $1/T$. We recover the desired result at $T = 0$; however, we have to stress out that in this model both limits $T \to 0$ and $V \to \infty$ do not commute.

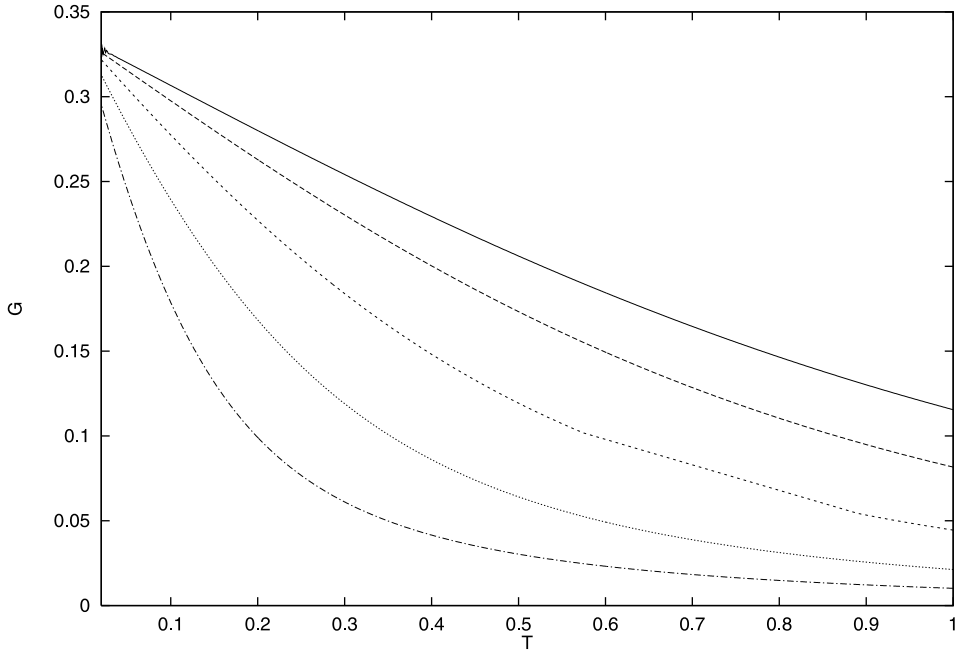

Figure 5. Parameter G for the 1D Ising spin glass for lengths $V = 2, 4, 8, 16, 32$ (from top to bottom).

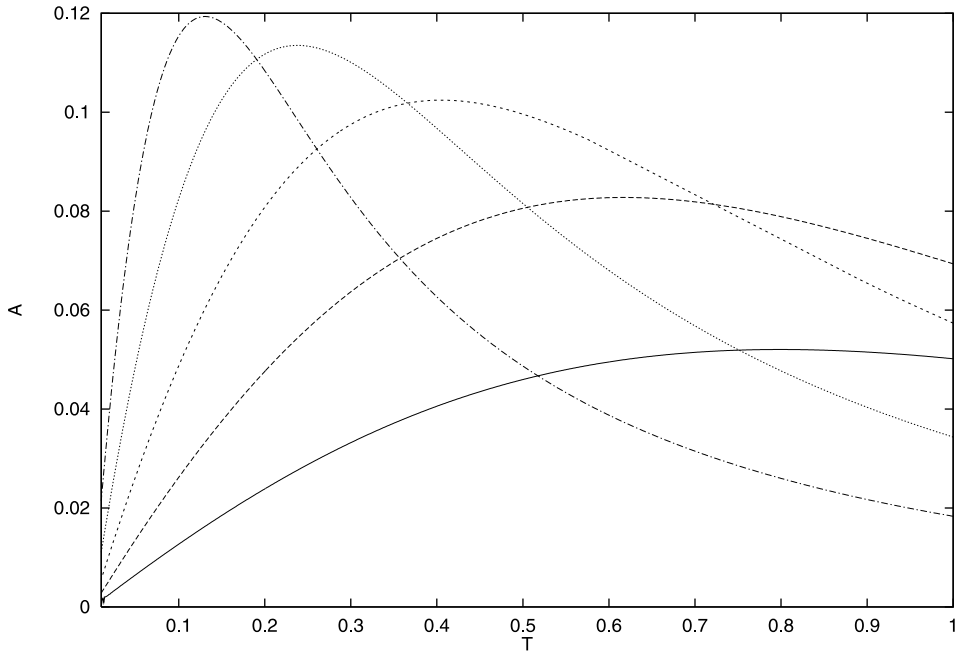

Figure 6. Parameter A for the 1D Ising spin glass for lengths $V = 2, 4, 8, 16, 32$ (from right to left).

6. The spherical Sherrington–Kirkpatrick spin glass

In this section we present some numerical simulations for the values of G and A in the Sherrington–Kirkpatrick spherical spin glass. This case is quite interesting because its low-temperature behaviour corresponds to the second possibility mentioned in section 2 where OPF vanish (in the $V \to \infty$ limit) much slower than the paramagnetic example studied in the previous section. Correspondingly, the study of OPF in this model turns out to be very complicated because the equilibrium solution is marginally stable. The model is defined by [13]

$$\mathcal{H} = -\sum_{i<j} J_{ij}\sigma_i\sigma_j \tag{66}$$

where $-\infty < \sigma_i < \infty$ and the values of σ_i satisfy the spherical global constraint $\sum_{i=1}^{N} \sigma_i^2 = N$. The couplings have an average of zero and a variance of $1/N$. The statics of this model can be solved with and without replicas [13]. In the former case one finds a transition at a temperature $T_c = 1$ where the Edwards–Anderson parameter is different from zero and equal to $1 - T$. In the latter case the transition corresponds to a macroscopic condensation of spin configurations onto the eigenvector corresponding to the largest eigenvalue. In the replica framework it has been shown [14] that the replica symmetric solution is the only possible one within the Parisi scheme. Since OPF vanish, the computation of G requires knowledge of finite-size corrections in the numerator and denominator in (5). A simple calculation reveals that the replica symmetric solution is marginally stable (the replicon eigenvalue vanishes everywhere below T_c) so the spin-glass susceptibility diverges. The situation is similar to what happens in the usual Sherrington–Kirkpatrick model with Ising spins. There the spin-glass susceptibility diverges proportionally to the volume, while now the divergence is much slower (such as $N^{1/3}$). This is so because in the present model OPF vanish like $N^{-2/3}$, while in the original SK model OPF are finite.

Again, to compute G we need to know the precise value of the amplitudes entering in the finite-size corrections in the parameters $\overline{\langle q^2\rangle}$, $\overline{\langle q^2\rangle^2}$, $\overline{\langle q^4\rangle}$. It is well known that analytic calculations of finite-size corrections in spin glasses are extremely difficult, especially for the amplitudes which are the quantities we are interested in. For the SK model these amplitudes are partially known only for some quantities [15]. For the present case we will use theoretical considerations and numerical simulations to estimate the asymptotic behaviour of the different overlaps.

We have simulated model (66) with a Monte Carlo dynamics where a change of a randomly chosen spin is proposed $\sigma_i \to \sigma_i + \delta r_i$, where δ is a constant number typically of order 1 and r_i is a random number uniformly distributed between $-\frac{1}{2}$ and $\frac{1}{2}$. The value of δ is chosen to have a reasonable acceptance rate. The value of all other spins is recalculated in order to satisfy the global spherical constraint. Moves are accepted according to the Glauber algorithm. Note that although we need to recalculate the value of all spins (changing them by multiplying by a normalization constant) the change in the energy can be simply calculated in a finite number of operations independent of N and simulations are as fast as with Ising spins. Our investigation has focused on small sizes, which reveal how G is a powerful tool to investigate phase transitions. The number of samples simulated are typically several thousand for very small sizes ($N = 4, 6, 8, 12, 16$) and several hundred for larger ones ($N = 24, 32, 40, 48, 64$). Overlaps have been computed by collecting statistics over a large time window (typically of the order of 10^5 Monte Carlo steps for each sample). We have evaluated $\overline{\langle q^2\rangle}^2$, $\overline{\langle q^2\rangle^2}$, $\overline{\langle q^4\rangle}$ for different sizes and temperatures.

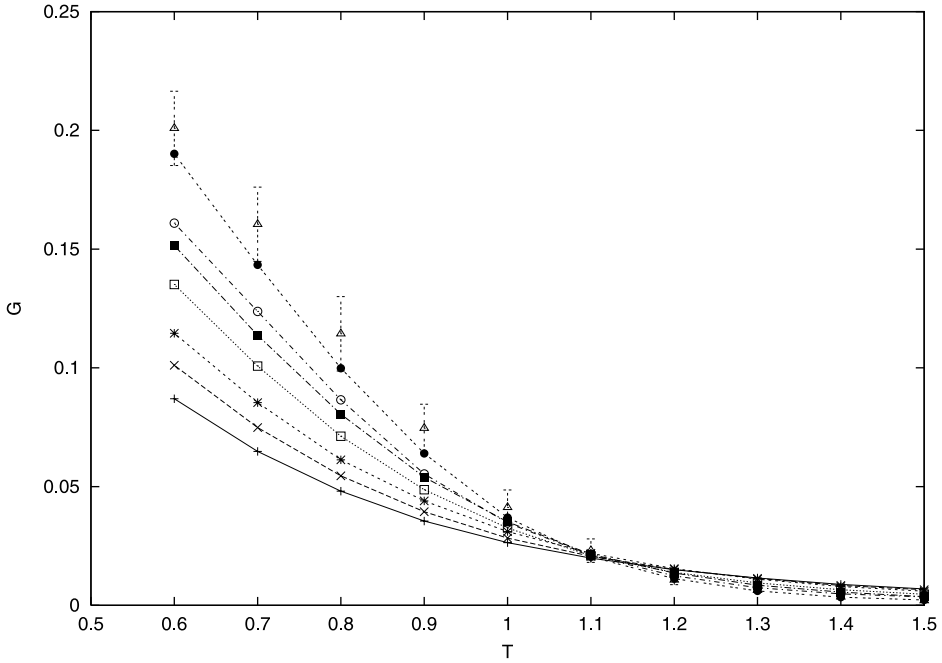

Figure 7. Parameter G for the SK spherical spin glass ($N = 4, 6, 8, 16, 24, 32, 48, 64$ from top to bottom at low temperatures). The largest error bars are shown for the largest size $N = 64$.

Figure 7 shows the results for G. Note that already for the smallest sizes there is a crossing of the different curves. The crossing appears for values of T well above $T_c = 1$ for the smallest sizes and moves to lower temperatures as the size increases converging to the expected value $T_c = 1$. It is quite surprising that already for very small sizes the transition can be clearly seen. The crossing moves down in temperature as the sizes increase and already for several tens of spins converges to the correct value $T = 1$. As a comparison we show in figure 8 the behaviour of the usual Binder parameter defined as

$$B = \frac{1}{2}\left(3 - \frac{\overline{\langle q^4\rangle}}{\overline{\langle q^2\rangle}^2}\right). \tag{67}$$

In this case the crossing point appears at low temperatures for small sizes and moves up very slowly as the size increases. However, already for the largest sizes the crossing is still at $T \simeq 0.8$ quite far from $T = 1$. A similar effect has been observed in simulations of the Sherrington–Kirkpatrick model with Ising spins [7, 16]. These results indicate that a numerical study of the parameter G can be extremely useful for locating phase transitions in disordered systems by studying very small sizes [17].

To analyse better the behaviour of G at low temperatures we have tried to extrapolate G to the large-N limit. Below T_c we expect for all three quantities $\overline{\langle q^2\rangle}$, $\overline{\langle q^2\rangle^2}$, $\overline{\langle q^4\rangle}$ the following finite-size corrections:

$$\overline{\langle q^2\rangle}^2, \overline{\langle q^2\rangle^2}, \overline{\langle q^4\rangle} = q_{EA}^4 + \frac{a}{N^{2/3}} + \frac{b}{N} + \frac{c}{N^{4/3}} + \frac{d}{N^{5/3}} \tag{68}$$

with $q_{EA} = 1 - T$. From these expressions we expect for G the following behaviour:

$$G = G_\infty + \frac{A}{N^{1/3}} + \frac{B}{N^{2/3}} + \mathrm{O}(1/N). \tag{69}$$

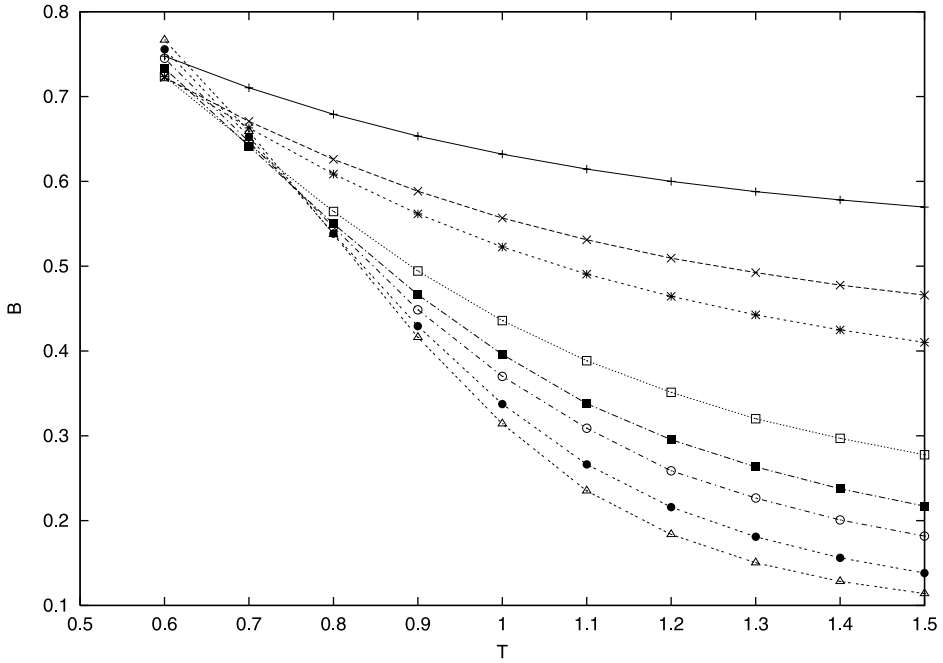

Figure 8. Binder cumulant B for the SK spherical spin glass ($N = 4, 6, 8, 16, 24, 32, 48, 64$ from top to bottom at low temperatures). Error bars are now negligible.

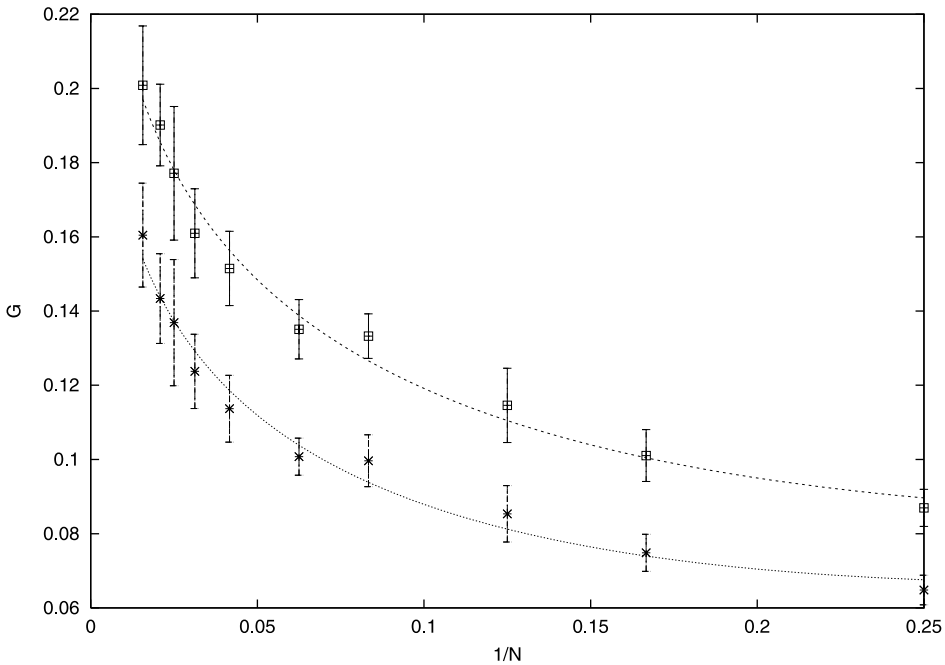

Figure 9. Fitting function (69) to the G parameter for different sizes at $T = 0.6$ (above) and $T = 07$ (below). Extrapolations to $N \to \infty$ are compatible with $G(V \to \infty) = \frac{1}{3}$ in the spin-glass phase.

We have fitted the values of G to this expression with G_∞, A, B as fitting parameters. The results and the fits are shown in figure 9. The extrapolated values for the lowest temperatures $T = 0.6, 0.7$ are $G_\infty(T = 0.6) = 0.34 \pm 0.2$ ($A(T = 0.6) = -0.71 \pm 0.1$ and $B(T = 0.6) = 0.49 \pm 0.13$), $G_\infty(T = 0.7) = 0.29 \pm 0.2$ ($A(T = 0.7) = -0.66 \pm 0.1$ and $B(T = 0.7) = 0.49 \pm 0.12$). Within errors these are compatible with the value $\frac{1}{3}$. Trying to have an estimate of G_∞ at higher temperatures is very difficult because critical effects are strong.

We must conclude that for this model the universal value of $\frac{1}{3}$ is well compatible with the data, suggesting that this may be a generic result for a spin-glass phase. Still we should do more extensive simulations to reach a final conclusion. Although going to larger sizes at the lowest temperatures may be possible this would require much longer computational times.

7. Outlook and discussion

In this paper we have investigated order parameter fluctuations in spin glasses. In particular, we have considered four different parameters: G, A for disconnected thermal averages and G_c, A_c for connected thermal averages. It has been shown recently that these models can be very useful in investigating phase transitions in disordered systems [4, 5] and several recent numerical works (Bokil *et al* in [4] and [6–8]) indeed support this conclusion. In this work we have concentrated our attention on obtaining general results and on applying them to certain solvable cases where these can be checked explicitly.

We have demonstrated that for models with a unique ground state and no gap in the ground-state local field distribution (for instance, all discrete models with continuous disordered couplings taken from a distribution without gap) G and G_c take the respective universal values $G = \frac{1}{3}$, $G_c = \frac{13}{31}$ at zero temperature for any finite volume. This is consequence of the dominance of one-spin excitations in OPF. For infinite volume this result still holds only in the regime where the limit $T \to 0$ is taken before the limit $V \to \infty$ and fast enough such that $TV \to 0$. This result has then been checked by calculating OPF in an instructive example without many-body interactions and for the case of the one-dimensional Ising spin glass where explicit computations can be done using the transfer matrix method. All these *good* properties suggest that both parameters G, G_c are ideal candidates to investigate phase transitions in disordered systems much like the Binder cumulant is for ordered systems.

The extension of this result to the other limit where $V \to \infty$ is taken before $T \to 0$ or, more generally, the limit $V \to \infty$ for T finite is far from trivial. In this last case, $G(V, T)$ is no longer volume independent. So the question is whether $G(V, T)$ converges in the large-V limit to the universal temperature-independent value $\frac{1}{3}$. At finite temperatures there are different possible scenarios for the value of G. In the case where OPF are finite in the $V \to \infty$ limit stochastic stability arguments and replica equivalence suggest that G should be $\frac{1}{3}$ everywhere in the spin-glass phase. Replica equivalence is a very generic property which, to the best of our knowledge, has not been emphasized before in the present context and implies that the free energy of a replicated disordered system must be proportional to the number of replicas. Note that at zero temperature replica equivalence cannot be used because the limits $V \to \infty$ and $T \to 0$ may not commute in that case. Actually, as we proved in section 4 only for models with a unique ground state and the absence of a gap in the fields distribution, does G takes the universal value $\frac{1}{3}$ but vanishes (exponentially fast with $1/T$) in the presence of a finite gap in that distribution.

The other interesting case is when OPF vanish. And here we can offer only more speculative arguments. A possible scenario is that which distinguishes two possibilities

depending on whether, in the infinite-volume limit, OPF vanish like $1/V$ or slower like $1/V^{\alpha}$ with $\alpha < 1$. If OPF vanish like $1/V$, G may take the value 0 typical of a paramagnetic phase (for instance, the case of the one-dimensional spin-glass model) or a temperature-dependent value (the instructive example of section 3). For these two solvable cases the parameter G is quite different. In the one-dimensional Ising spin glass we find $G = \frac{1}{3}\delta_{T,0}$, while in the instructive example we find $G = \hat{G}(T)$, with $\hat{G}$ a monotonically decreasing function of T with $\hat{G}(0) = \frac{1}{3}$. The reason for these two different behaviours in a disordered phase may be ascribed to the fact that, in the first case, there is a critical point at $T = 0$, while in the second there is no critical point at all. So G is a good indicator for a phase transition. However, this observation must be taken with caution because the parameter G_c shows a different behaviour for the instructive example $G_c = \frac{13}{31}\delta_{T,0}$ similar to the behaviour of G in the one-dimensional spin glass. We expect the interesting behaviour to be present in models where OPF vanish like $1/V^{\alpha}$ with $\alpha < 1$. This class of models includes disordered systems where the replica symmetric solution is marginally stable and eventually finite-dimensional spin glasses if replica symmetry is not broken, a question which is still unsolved [18]. This case is much more subtle because replica equivalence cannot be used (nor probably the stochastic stability property) and finite-size corrections must be known. To address this question we have performed a numerical study of the spherical Sherrington–Kirkpatrick spin glass. There are two main outcomes: (a) the parameter G is an excellent tool for locating the spin-glass transition already for very small sizes (more precise than the usual Binder parameter) and (b) an infinite-volume numerical extrapolation (compatible with the expected form for the finite-size corrections) of the value of G in the spin-glass phase is well compatible with the value $\frac{1}{3}$.

Before concluding we want to stress that, apart from their applicability to the study of spin-glass transitions, OPF are interesting quantities which deserve further investigation. The outcome of the proof in section 4 is that OPF are very sensitive and rely completely on the effect of rare samples. Actually, rare samples are those which induce the largest OPF and fix the value of G to $\frac{1}{3}$. A comprehensive study of rare events in disordered systems is still missing. Averaging of extensive quantities such as the replicated free energy in standard renormalization group approaches may wipe out a large number of effects such as those discussed here. Certainly more detailed investigations are needed to clarify the situation. Although a final theorem which resolves this problem may be at hand, we think that the search for non-trivial counterexamples of the different possibilities discussed in this paper could be very useful.

Acknowledgments

We acknowledge discussions with M Picco and A J Bray. We are indebted to A A Garriga and A Rocco for a careful reading of the manuscript. FR is supported by the Ministerio de Educación y Ciencia in Spain (PB97-0971). MS is supported by the Ministerio de Educación y Ciencia of Spain, grant AP-98 36523875.

References

[1] Mézard M, Parisi G and Virasoro M A 1987 *Spin Glass Theory and Beyond* (Singapore: World Scientific)
Binder K and Young A P 1986 *Rev. Mod. Phys.* **58** 801
Fischer K H and Hertz J A 1991 *Spin Glasses* (Cambridge: Cambridge University Press)
[2] Guerra F 1996 *Int. J. Mod. Phys.* B **10** 1675
[3] Franz S, Parisi G, Mézard M and Peliti L 2000 *J. Stat. Phys.* **97** 459
(Franz S, Parisi G, Mézard M and Peliti L 1999 *Preprint* cond-mat/9903370)

[4] Marinari E, Naitza C, Parisi G, Picco M, Ritort F and Zuliani F 1998 *Phys. Rev. Lett.* **81** 1698
Bokil H, Bray A J, Drossel B and Moore M A 1998 *Preprint* cond-mat/9811080
Marinari E, Naitza C, Parisi G, Picco M, Ritort F and Zuliani F 1999 *Phys. Rev. Lett.* **82** 5175
(Marinari E, Naitza C, Parisi G, Picco M, Ritort F and Zuliani F 1998 *Preprint* cond-mat/9811304)
[5] Parisi G, Picco M and Ritort F 1999 *Phys. Rev.* E **60** 58
[6] Hukushima H and Kawamura K 2000 Chiral-glass transition and replica symmetry breaking of three-dimensional Heisenberg spin glasses *Preprint* cond-mat/0001127 (*Phys. Rev.* E, at press)
[7] Hukushima K and Kawamura H 2000 How the replica-symmetry-breaking transition looks like in finite-size simulations *Preprint* cond-mat/0003226
[8] Pagnani A, Parisi G and Ricci-Tersenghi F 2000 *Phys. Rev. Lett.* **84** 2026
[9] Mézard M, Parisi G, Sourlas N and Virasoro M A 1984 *J. Physique* **45** 843
[10] Bray A J, Moore M A and Young A P 1983 *J. Phys. A: Math. Gen.* **16** 2063
[11] Parisi G 1980 *J. Phys. A: Math. Gen.* **13** 1101
(Parisi G 1998 *Preprint* cond-mat/9801081)
[12] Bray A J and Moore M A 1985 *J. Phys. A: Math. Gen.* **18** L683
[13] Kosterlitz J M, Thouless D J and Jones R C 1976 *Phys. Rev. Lett.* **36** 1217
[14] Jagannathan A and Rudnick J 1989 *J. Phys. A: Math. Gen.* **22** 5131
[15] Parisi G, Ritort F and Slanina F 1993 *J. Phys. A: Math. Gen.* **26** 247
Parisi G, Ritort F and Slanina F 1993 *J. Phys. A: Math. Gen.* **26** 3775
[16] Bhatt R N and Young A P 1985 *Phys. Rev. Lett.* **54** 924
[17] Picco M, Ritort F and Sales M work in progress
[18] Marinari E, Parisi G, Ricci-Tersenghi F, Ruiz-Lorenzo J J and Zuliani F 2000 *J. Stat. Phys.* **98** 973
(Marinari E, Parisi G, Ricci-Tersenghi F, Ruiz-Lorenzo J J and Zuliani F 1999 *Preprint* cond-mat/9906076)
[19] Palassini M and Young A P 2000 The nature of the spin glass state *Preprint* cond-mat/0002134 (*Phys. Rev. Lett.* at press)
Krzakala F and Martin O 2000 *Preprint* cond-mat/0002055