A new method to compute the configurational entropy in glassy systems

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Abstract. We propose a new method to compute the configurational entropy of glassy systems as a function of the free energy of valleys at a given temperature, in the framework of the Stillinger and Weber approach. In this method, which we call free-energy inherent structures (FEIS) approach, valleys are represented by inherent structures that are statistically grouped according to their free-energy rather than the energy as is commonly done in the standard procedure. The FEIS method provides a further step toward a description of the relaxational behavior of glassy systems in terms of a free energy measure. It can be used to determine the character of the glass transition as well as the mode coupling and the Kauzmann temperatures. We illustrate the usefulness of the method by applying it to simple models of glasses and spin glasses.

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1 Introduction

Spin glasses and structural glasses are characterized by the presence of a complex structure of stable and metastable states [1]. In particular, the free energy landscape is characterized by a large number of valleys which in spin-glass theory are also commonly referred to as basins, pure states, phases or ergodic components. These valleys contain a large number of configurations (typically growing exponentially with the size of the system) with macroscopic properties (for example the energy or the magnetization) that in general depend on the specific valley. The complexity of the configurational space topology reflects itself into a complex dynamical behavior commonly referred to as *glassy behavior*. These ideas trace back to more that 30 years ago to a seminal paper of Goldstein [2], who suggested that the dynamics of a supercooled liquid can be understood in terms of a diffusive process between different valleys. At low temperature the dynamics slows down since the system gets trapped for long time in a valley and the slow long time relaxation is only governed by the inter-valley motion.

Along the same lines, but in a different context, Stillinger and Weber (hereafter referred as SW) proposed in the early eighties to identify each valley with its minimum, called Inherent Structure (IS) and to build up an IS-based analysis [3]. Each valley contains all those configurations that map into the IS by a steepest descent dynamics. On the one hand, such a coarse-grained description of the phase space may be useful to grasp the universal and generic features of glassy dynamics. On the other hand, replacing each valley with a single configuration implies of course a strong reduction of information. A relevant question then is to understand under which conditions the resulting IS-based dynamics is equally well representative of the off equilibrium behavior of the system. From purely theoretical grounds, the decomposition of the phase space into non-overlapping valleys is always possible. However, its operative definition may be a rather subtle issue. In mean-field theory, where ergodicity breaking holds, the decomposition of the phase space into valleys has a clear physical meaning. In that case one can define as configurations belonging to the same valley those such that starting from any of them, any other configuration in the same valley can be reached (or get close as we like for continuous systems) in a finite time. In the case of short ranged systems, however, the extension of this definition remains quite unclear. In fact, in the case of finite

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dimensional systems, even in presence of Replica Symmetry Breaking (RSB), activated processes must be included in the physical picture.

An alternative point of view rests on a dynamical definition of the concept of valley [4]. Metastable states or valleys $\mathcal{V}$ can be defined by introducing the observation time τ and looking at the cumulative probability $P^{\mathcal{V}}(\tau)$ that the system starting in any configuration contained in the valley $\mathcal{V}$ at time $t = 0$ escapes from $\mathcal{V}$ at or before time τ. The valley is well defined [5] if there exists a reasonably small significance level p such that the following inequality is satisfied:

$$P^{\mathcal{V}}(\tau) \le p. \tag{1}$$

The escape probability, and hence the partition, in general depends on the external parameters such as fields or temperature and on the system size N. If for a valley it happens that

$$\lim_{\tau \to \infty} \lim_{N \to \infty} P^{\mathcal{V}}(\tau) = 0 \tag{2}$$

then the valley is absolutely confined [5] in the thermodynamic limit and corresponds to an ergodic component. This is the typical case for mean-field models since free-energy barriers between valleys growth with the system size.

For non-mean-field systems valleys are not, in general, absolutely confined and their identification is not trivial. A possible strategy to deal with those systems is that of looking for possible simple limiting cases and using them to partition the phase space. The SW scheme belongs to this class. Indeed since at $T = 0$ any barrier cannot be surmounted, it is clear that all valleys are absolutely confined at $T = 0$, making their identification simpler. The SW scheme identifies valley with a $T = 0$ dynamics, therefore we can regard the SW scheme as a $T = 0$ partitioning.

In the original SW scheme different valleys are classified according to the energy of the minimum (IS). This picture can be somewhat misleading since it plays down the role of entropy. In this paper we shall discuss the more physical classification in terms of *Free Energy Inherent Structure* (FEIS). We also introduce a direct method, which to our knowledge is new, of computing the free energy of valleys. We emphasize that the FEIS classification is more general than the usual IS-energy one. The two classifications lead to the same information only if different valleys have similar entropies, which in general may not be the case.

Strictly speaking, the partitioning depends on temperature, this is particularly relevant for the dynamical properties of the systems. We do not address here this problem since we are interested in understanding the role of entropy once a partition is given. For this reason we merely assume the validity of the SW scheme which has the advantage of being quite easy to be implemented.

The paper is organized as follows. In Section 2 we discuss the phase space partitioning and identify the relevant physical quantities. The method to compute the FEIS is described in Section 3 and is applied to two representative models, the Sherrington-Kirkpatrick (SK) model and

the Random Orthogonal (ROM), in Sections 4 and 5. The choice of these model is motivated by their different phase space organization. Finally Section 6 contains conclusions and some perspectives.

2 Partitioning the phase space into valleys: the free-energy landscape

In general, given a decomposition of the phase space into non-overlapping valleys, we can write the partition function $\mathcal{Z}$ as

$$\mathcal{Z}(T) = \sum_{\mathcal{C}} \exp\left(-\beta \mathcal{H}(\mathcal{C})\right) = \sum_{\mathcal{V}} \exp\left(-\beta \mathcal{F}_{\mathcal{V}}(T)\right), \tag{3}$$

where $\mathcal{C}$ denotes the spin configurations, $\mathcal{H}$ is the Hamiltonian and $\beta \equiv \frac{1}{T}$ is the inverse temperature. $\mathcal{F}_{\mathcal{V}}(T)$ is the free energy of the valley $\mathcal{V}$,

$$\mathcal{F}_{\mathcal{V}}(T) \equiv -\frac{1}{\beta} \log \left(\sum_{\mathcal{C} \in \mathcal{V}} \exp(-\beta \mathcal{H}(\mathcal{C})) \right). \tag{4}$$

Expectation values of observables can be defined in a given valley $\mathcal{V}$ by restricting the Boltzmann measure to configurations belonging to that valley (restricted ensemble [5]):

$$\langle \mathcal{A} \rangle_{\mathcal{V}} \equiv \sum_{\mathcal{C} \in \mathcal{V}} \mathcal{A}(\mathcal{C}) \exp(-\beta \mathcal{H}(\mathcal{C}) + \beta \mathcal{F}_{\mathcal{V}}(T)). \tag{5}$$

Note that

$$\langle \mathcal{A} \rangle = \sum_{\mathcal{V}} \langle \mathcal{A} \rangle_{\mathcal{V}} \exp\left(-\beta \mathcal{F}_{\mathcal{V}}(T) + \beta \mathcal{F}(T)\right), \tag{6}$$

where $\mathcal{F}$ is the total free energy of the system. After these definitions it is natural to consider the entropy of the valley $\mathcal{V}$, defined as

$$S_{\mathcal{V}}(T) \equiv \beta(\langle E \rangle_{\mathcal{V}}(T) - \mathcal{F}_{\mathcal{V}}(T)). \tag{7}$$

In principle the partitioning of the phase space into valleys allows to extend all thermodynamic relations to more general valley-dependent ones. As stated above, the relevant question is whether a given partitioning of phase space has a physical meaning.

Recent results about the dynamics of spin glasses have shown that a modified form of the fluctuation-dissipation theorem (hereafter referred to as FDT) is satisfied in the aging regime [6]. For structural glasses or one-step RSB spin glasses these violations are asymptotically described by a single time-scale which can be related to an effective temperature. Violations of FDT are tightly related to the spectrum of off-equilibrium fluctuations and the dependence on a single effective temperature has been advocated as the consequence of the cooperative character of the dynamics [7]. Although FDT violations have been computed in detail only in mean-field systems there is evidence that they yield a physically valid description of the free energy fluctuations in the aging state also for short-ranged systems [8]. The fact that FDT violations can be

well rationalized in a mean-field framework [9] (the effective temperature is related to the function $x(q)$ in the Parisi solution of spin glasses) suggests that some features of the mean-field theory can be extended to realistic systems [7]. A key concept describing this mean field behavior is the *configurational entropy* (also called *complexity*) $\mathcal{S}_c(f,T)$ defined as the number of valleys with a given free energy per site f. The configurational entropy counts the number of valleys accessible to the system in the same way as the usual entropy in Boltzmann theory counts the number of configurations with a given energy. Therefore, the information that it contains has physical meaning if an equiprobability hypothesis (equivalent to that of equilibrium ensemble theory) holds for spin glasses and glasses in the off-equilibrium regime [7]. This hypothesis assumes that valleys with a given free energy f have the same weight and can be treated on the same footing as far as the dynamical properties of the system are concerned. The implications of such an assumption for the description of complex landscapes in glassy systems are very strong. It provides a flat measure for the dynamics of glassy systems similar to the Edwards measure for granular media [10,11].

In this framework a description of the off-equilibrium dynamics in terms of the complexity has been successfully obtained for structural glass models [12] within the IS formalism [3] where each valley is identified by its minimum IS. The physical assumption behind the validity and usefulness of this coarse grained description (where configurations are grouped into different IS) is that the time-scale of inter-valley motion is much larger than the time-scale of intra-valley motion. If typical valleys are locally similar, *i.e.*, they can have different energies but similar entropies, then one may simply count them from the probability distribution of the IS energies and obtain the complexity, apart from an unknown constant. This last assumption can be relaxed by estimating the entropies of the valleys by treating fluctuations with the harmonic approximation [13–18], or by more realistic approximations which take anharmonicity into account (unfortunately this procedure is not applicable to discrete systems). It should be noted that that such a method for evaluating the complexity in structural glasses stems out naturally from a recently proposed thermodynamical approach [19,20,13] to the liquid glass transition, within the approximation that free energy valleys are well described by the corresponding IS valleys.

We note that the utility of the SW decomposition is less evident in the case of Full Replica Symmetry Breaking (FRSB) spin glasses where the structure of valleys is more sensitive to temperature and no clear time scale separation exist, making the application of a $T = 0$ decomposition to finite T questionable. Nevertheless a recent numerical study [21] shows that the coarse graining from configurations to IS preserves the physical properties of the system. We shall see that a statistical description of the free-energy landscape made in terms of the free energy of valleys (rather than their energy) is still useful also for FRSB spin glasses at finite temperature, and that the cor-

responding complexity $\mathcal{S}_c(f,T)$ gives a proper description of the glassy phase.

In the next section we shall propose a method to numerically compute the valley free energy suitable for discrete systems. This method will provide us with the explicit dependence of the configurational entropy on both temperature and free energy. Moreover it directly gives $\mathcal{S}_c$ (including also undetermined global constants) without using any approximation for the intra-valley entropy (such as the harmonic approximation discussed in the last but one paragraph), improving the results obtained with other methods [13–18,22]. To our knowledge this is the first time that a method to compute the statistical distribution of the free energies of the IS valleys has been proposed and tested.

3 Description of the free-energy inherent structures (FEIS) method

We consider the IS decomposition introduced by Stillinger and Weber (SW) [3], where each valley $\mathcal{V}$ is labeled by the corresponding minimum (IS), and denote its free energy per site by

$$f_{\text{IS}} \equiv \frac{1}{N}\mathcal{F}_{\mathcal{V}}. \tag{8}$$

Hereafter small letters will denote intensive quantities.

Our goal is to compute the complexity $\mathcal{S}_c(f,T)$ without making any assumption on the similarity of valleys. In the context of Lennard-Jones glasses, Speedy [23] has proposed to compute the free energy of a valley by adding to the Hamiltonian a coupling term between the configuration that labels the IS and the run-time configuration, $-\epsilon q$, q being an appropriately defined overlap. A similar approach in which the complexity is evaluated by coupling the run-time configuration to a generic configuration of the valley was considered in the first reference in [13]. By taking the thermodynamic limit first and extrapolating later to $\epsilon \to 0$ it is possible to restrict the measure to those configurations $\mathcal{C}$ belonging to the IS valley. This procedure is laborious, since it requires extensive simulations for different values of the coupling ϵ and for each different IS.

Here we propose a different strategy based on the probabilistic definition [24] of the valley free energy. The dynamical evolution of the system defines a probability measure $p_{\mathcal{V}}$ over the valleys. In the case of an ergodic dynamics, and assuming that the observation time is $\tau_{tot} \gg \tau_{eq}$, the statistical weight of the single valley is obtainable directly from (3) and the Boltzmann *a priori* equiprobability hypothesis [24]:

$$p_{\mathcal{V}}(T) = \frac{\tau_{\mathcal{V}}}{\tau_{tot}} = \exp\left(-\beta\mathcal{F}_{\mathcal{V}}(T) + \beta\mathcal{F}_{\text{eq}}(T)\right), \tag{9}$$

where $\tau_{\mathcal{V}}$ denote the time spent by system in the valley $\mathcal{V}$ during the total observation time τ_{tot}, and $\mathcal{F}_{\text{eq}}(T)$ the equilibrium free energy. Alternatively equation (9) can be derived from the information theory as the ensemble which minimizes the information to specify one valley when we

only know that the system is in contact with a heat bath at T (*unbiased component ensemble*) [5]. In either case the probability to find at temperature T an IS with free energy density equal to f is given by

$$\mathcal{P}(f,T) = \langle\delta(f - f_{\mathrm{IS}})\rangle = \sum_{\mathrm{IS}} \delta(f - f_{\mathrm{IS}}) \ p_{\mathrm{IS}}(T)$$

$$= \frac{g(f,T)\exp(-\beta N f)}{\sum_{\mathrm{IS}}\exp(-\beta N f_{\mathrm{IS}})} \ , \qquad (10)$$

where $g(f,T)$ is the density of IS with free energy density f which defines the extensive complexity

$$\mathcal{S}_c(f,T) \equiv \log(g(f,T)), \qquad (11)$$

and $p_{\mathrm{IS}}(T)$ is given by (9). The denominator in (10) is the equilibrium partition function

$$\mathcal{Z}(T) = \exp(-\beta N f_{\mathrm{eq}}(T)). \qquad (12)$$

Equations (10)-(12) lead to the relation

$$s_c(f,T) = \frac{\log\left[\mathcal{P}(f,T)\right]}{N} + \beta(f - f_{\mathrm{eq}}(T)) \ . \qquad (13)$$

The key formula in this expression is the probability $\mathcal{P}(f,T)$ which can be estimated by computing f_{IS} from (9) with the following procedure. After having thermalized the system at temperature T for t_{therm} Monte Carlo (MC) steps, a steepest descent procedure is used every t_{run} MC steps for N_{run} to identify the IS [25]. The interval t_{run} is chosen to be of the same order as t_{therm} to ensure that configurations obtained at the end of each period are uncorrelated.

If the number of different IS is not too large and N_{run} is taken large enough to ensure that each IS has been visited a substantial number of times, then p_{IS} can be estimated as

$$p_{\mathrm{IS}}(T) = \frac{N_{\mathrm{IS}}}{N_{\mathrm{run}}} \qquad (14)$$

where N_{IS} is the number of times the given IS has been found ($\sum_{\mathrm{IS}} N_{\mathrm{IS}} = N_{\mathrm{run}}$). From (9) the IS free energy now reads

$$f_{\mathrm{IS}}(T) = -\frac{T}{N}\log\left(\frac{N_{\mathrm{IS}}}{N_{\mathrm{run}}}\right) + f_{\mathrm{eq}}(T). \qquad (15)$$

The equilibrium free energy $f_{\mathrm{eq}}(T)$ can be computed by performing a different MC run and integrating the energy of the system from infinite temperature limit down to the working temperature T:

$$\beta f_{\mathrm{eq}}(T) = \int_0^\beta \mathrm{d}\beta' e_{\mathrm{eq}}(\beta') - s_{\mathrm{eq}}(\beta = 0). \qquad (16)$$

Finally from the value of f_{IS} it is easy to construct the histogram $\mathcal{P}(f,T)$ and using equation (13) compute $s_c(f,T)$.

This approach has an important difference with the usual SW decomposition. In the standard SW method IS with the same energy e_{IS} are assumed to occur with the same probability. However, in the FEIS method IS with the same free energy f_{IS} are grouped together. Compared to (10), in the standard SW procedure we have:

$$\mathcal{P}(e,T) = \langle\delta(e - e_{\mathrm{IS}})\rangle = \sum_{\mathrm{IS}} \delta(e - e_{\mathrm{IS}}) \ p_{\mathrm{IS}}(T)$$

$$= \frac{g_e(e)\exp(-\beta N f(e,T))}{\sum_{\mathrm{IS}}\exp(-\beta N f_{\mathrm{IS}}(e,T))} \qquad (17)$$

and therefore

$$s_c(e) = \frac{\log\left[\mathcal{P}(e,T)\right]}{N} + \beta(f(e,T) - f_{\mathrm{eq}}(T)) \qquad (18)$$

with

$$s_c(e) = \lim_{T\to 0} s_c(f,T). \qquad (19)$$

For models with continuous degrees of freedom $s_c(e)$ can be obtained directly from (18) by evaluating $f(e,T)$ with, *e.g.*, the harmonic approximation.

For discrete models this decomposition is useful whenever the free energy of valleys with IS energy e has a trivial dependence on e:

$$f(e,T) \simeq e + f_0(T), \qquad (20)$$

with $f_0(T)$ only function of temperature. Note that in this case one has

$$s_c(f,T) = s_c(e + f_0(T)). \qquad (21)$$

This approach relies on the hypothesis that all valleys with the same IS energy have the same relevance to the statistical properties of the system, so that the frequency of visiting an IS with a given energy only depends on the total number of IS with that energy. If the approximation (20) is valid, $s_c(e)$ can be evaluated, apart from the unknown constant $f_0(T)$, directly from (18). As the unknown constant in $s_c(e)$ only depends on T (and not on the energy) one can check the correctness of the results from the superposition of the appropriately shifted curves obtained at different temperatures. Usually it is reasonable to expect that this happens in at least two different situations. First, when the temperature is low enough that only configurations near the bottom of the IS valleys contribute; second, when the IS-valleys are narrow as in REM-like models [26]. As we are going to discuss in detail, this is not the case in FRSB spin glasses, where the size of valleys must also be taken into account. In such case the configurational entropy is meaningful only when expressed in terms of the free energies of the valleys.

We conclude this section by noting that the partition function (12) can be written as

$$\mathcal{Z}(T) = \sum_{IS}\exp(-\beta N f_{\mathrm{IS}}) = \int \mathrm{d}f \ g(f,T)\exp(-\beta N f)$$

$$= \int \mathrm{d}f \ \exp(-\beta N \Phi(f,T)), \qquad (22)$$

with the generalized free energy

$$\Phi(f,T) \equiv f - T s_c(f,T). \qquad (23)$$

In the large N limit, the equilibrium free energy is given by the minimum of Φ:

$$f_{\text{eq}}(T) = \min_f \Phi(f, T) = f^*(T) - T\, s_c(f^*(T), T), \quad (24)$$

where we used (12) and (22). Under the assumption that the typical IS energy $e^*(T)$ is similar to the equilibrium energy $e_{\text{eq}}(T)$ then the complexity $s_c(f^*(T), T)$ is simply given by the difference between the entropy of the system at equilibrium $s_{\text{eq}}(T)$ and the typical IS entropy $s^*(T)$ (see Refs. [19,20]). This allows the numerical computation of $s_c(f^*(T), T)$ in systems with continuous degree of freedom such as structural glass models where $s^*(T)$ can be evaluated as the average entropy of a disordered harmonic solid (or also within more realistic approximations).

The formalism developed in [19,20] is appropriate for glassy systems with a clearcut time-scale separation between the inter-valley and the intra-valley motion, so that the valley free energy is a well defined quantity. Our approach does not suffer from this limitation and we shall show that Φ in (23) is the relevant quantity to look at also in FRSB model, where no clear time-scale separation exists at finite temperature. Moreover it is just the behavior of Φ at different temperatures which gives information on the nature of the glass transition allowing to predict the values of the different relevant temperatures characterizing the glass transition (*e.g.* the MCT transition temperature or the Kauzmann temperature).

In what follows, we will show the powerfulness of our method using simple spin models of glassy systems.

4 Models and simulation details

We have considered two spin glass models: the Sherrington-Kirkpatrick model [27] (SK) and the random orthogonal model (ROM) [28]. They are both described by the Hamiltonian

$$\mathcal{H} = - \sum_{1 \le i < j \le N} J_{ij}\, \sigma_i \sigma_j, \quad (25)$$

where the spins are Ising spins ($\sigma_i = \pm 1$) and the J_{ij} are symmetric ($J_{ij} = J_{ji}$) quenched random couplings. In the SK model the J_{ij} are uncorrelated variables with zero mean and $1/N$ variance, while in the ROM J_{ij} are the elements of a random orthogonal matrix, with $J_{ii} = 0$ and

$$\sum_k J_{ik} J_{jk} = 4\delta_{ij}. \quad (26)$$

We have considered both the SK model with binary couplings $J_{ij} = \pm 1/\sqrt{N}$ and with Gaussian couplings $P(J_{ij}) = (2\pi/N)^{-1/2} \exp(-N J_{ij}^2/2)$, obtaining very similar results.

The reason for this choice of the SK and ROM is based on the fact that they describe the two most relevant scenarios of mean-field glassy systems: the SK model gives the mean-field theory for disordered and frustrated magnets with FRSB, while the ROM describes structural glasses in the mode coupling approximation [1]. Recent work [22] suggests that the study of finite-sized mean-field systems is a useful route to investigate activated processes in real systems. A statistical analysis of the IS in the SK model has been presented in [21,22]. In particular, it was shown in [21] that the probability distribution of the overlap $P(q)$, *i.e.* the order parameter that describes the FRSB transition, can be computed between IS instead of equilibrium configurations (weighting the IS with their probability of occurrence in the simulation $p_{IS}(T)$, which is the weight of the corresponding basin at the considered temperature). In this sense, the coarse-graining from configurations to IS seems to preserve the physical properties of the system. For the ROM it has been found in [22] that valleys are statistically identical as they have a very small intra-valley entropy, and the usual SW decomposition in terms of the energy of the different IS provides a fairly good statistical description of the potential energy landscape and the relaxational dynamics. In the SK model (and, by extension, all models with continuous RSB), contrarily to the ROM, valleys can be very different, so the IS free energy has important contributions coming from intra-valley fluctuations.

We have considered small volumes, typically $N = 32$ and 64, to avoid having too many valleys. In fact the number of stationary points of the energy surface $\mathcal{N}_{\text{IS}}$ is known to grow exponentially with the system size:

$$\mathcal{N}_{\text{IS}} \sim \exp(\alpha N) \quad (27)$$

with $\alpha \simeq 0.2$ for the SK model [29] and 0.3 for the ROM [30]. Because of that, if we want to satisfy the condition $\mathcal{N}_{\text{IS}}/N_{\text{run}} \sim \mathcal{O}(1)$ in (14), N cannot be too large, otherwise $\mathcal{N}_{\text{IS}}/N_{\text{run}} = 0$ for those IS inefficiently sampled. In the case of the SK model for $N = 32$ we have $\mathcal{N}_{\text{IS}} \simeq 10^3$ while for $N = 64$ typically we have $\mathcal{N}_{\text{IS}} \simeq 10^5$. In all cases we used $N_{\text{run}} = 10^6$. In general, the study of larger sizes requires a very large amount of memory and CPU time though it should be possible, as we will discuss in more detail in the following, to restrict the analysis to a smaller range of free energy values.

We have also checked that, as expected [25], these results do not depend on the details of the algorithm used to determine the IS: we have verified that the greedy algorithm (which follows the steepest path in the phase space) and a $T = 0$ MC dynamics produce the same results. For the finite T simulations we have used a MC update with a simple Glauber dynamical rule. To reduce sample-to-sample fluctuations for the SK model data have been averaged over 10 samples. For the ROM we find very small sample-to-sample fluctuations. Already for systems of size $N = 32$ different samples almost give the same results. This is most probably due to the high degree of correlation among the couplings imposed by the orthogonality requirement. For this reason, and because simulations turn out to be very long, the data for ROM reported in the figures have been averaged over only two samples.
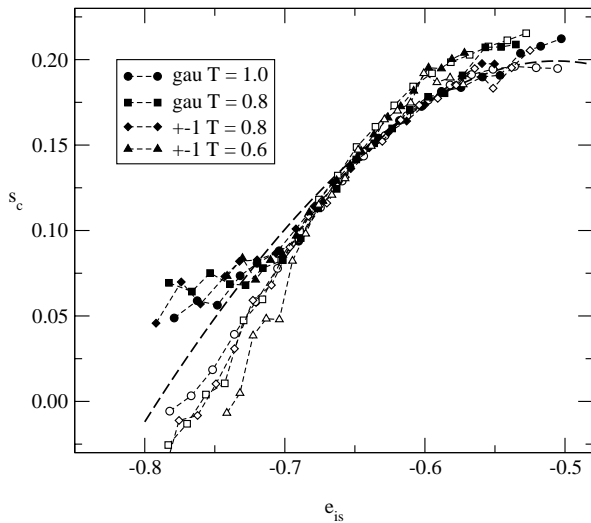
Fig. 1. The complexity as a function of the IS energy for the SK model with $N = 64$ at temperatures $T = 1.0, 0.8, 0.6$, for Gaussian and ± 1 couplings. The filled symbols are quenched averages, the empty ones correspond to annealed averages. The dashed line is the analytic annealed result [29].

5 Results and discussion

In Figure 1 we show the complexity $s_c(e)$ for the SK model as a function of the IS energy as defined in the usual SW decomposition computed from equation (18). We have considered two different averages:

- the annealed average, where we first average $\mathcal{P}(e,T)$ over the disorder (average denoted by $\overline{(...)}$), and the configurational entropy per spin is estimated as

$$s_c(e) \equiv \frac{\log(\overline{\mathcal{P}(e,T)})}{N} + \beta e + \text{const.}, \qquad (28)$$

- the quenched average, where

$$s_c(e) \equiv \frac{\overline{\log(\mathcal{P}(e,T))}}{N} + \beta e + \text{const.} \qquad (29)$$

In either case we have determined the normalization constant by superimposing the data to the Bray and Moore [29] analytical result, obtained within the annealed approximation. A reasonable estimate of the size of the error induced from sample to sample fluctuations is given from the dispersion of the curves at similar values of the temperature.

The annealed average corresponds to what is known as white average in the calculation of the number of TAP solutions. For the SK model, a zero-temperature calculation shows [29] that the white average gives incorrect results below a critical energy $e_c = -0.672$, where in fact the quenched average is needed. This can be well appreciated in Figure 1. Two results emerge from this figure:

- the two types of average agree above the predicted value for e_c, and clearly differ below. The strong difference found between the two kind of average reflects
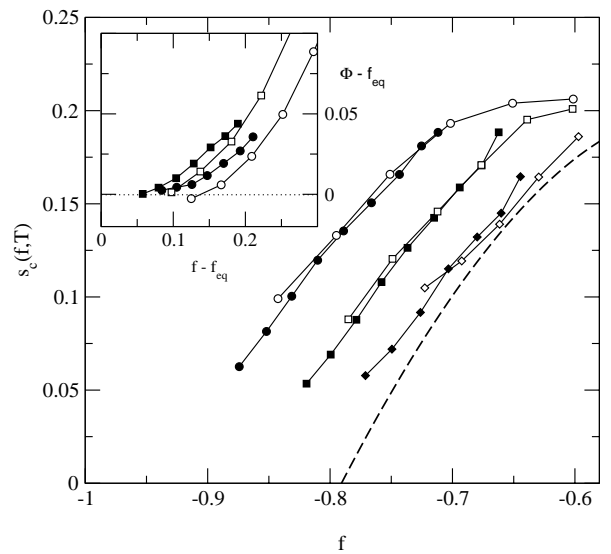
Fig. 2. Complexity for the SK model as function of the free energy for $T = 1.0$ (circles), 0.8 (squares), 0.6 (diamonds). Empty symbols correspond to $N = 32$, filled symbols to $N = 64$. The dashed line is the analytic result [29]. In the inset we plot the potential $\Phi(f,T) - f_{eq}(T)$ as function of $f - f_{eq}$.

the fact [29] that the IS minima are uncorrelated only for $e \geq e_c$ whereas below the breaking of replica symmetry should be taken into account;

- above e_c it is impossible to obtain a good collapse of the data, and they do not fit the theoretical prediction [29]. This effect, which is absent in the ROM [22] where all data collapse pretty well in a single curve, suggests that a complexity defined in terms of the usual SW decomposition does not give a good description of the free energy landscape of the SK model.

To compute the complexity as function of IS free energy we have estimated the IS free energy from (15) and evaluated the complexity using (13). We note that the finite number of searches introduces some ambiguity in the normalization constant. Indeed since N_{run} is finite the IS with probability

$$p_{\mathrm{IS}}(T) < p_{\mathrm{IS}}^0 = \exp(-\beta N(f_{\mathrm{IS}}^0 - f_{\mathrm{eq}}(T))) = \frac{1}{N_{\mathrm{run}}}, \quad (30)$$

i.e., with free energy $f_{\mathrm{IS}} > f_{\mathrm{IS}}^0$, are never found. Furthermore, one can assume that $p_{\mathrm{IS}}(T)$ is correctly evaluated only for IS that have been found at least few times (say 5 times). Consequently $P(f,T)$ is only known for $f < f_{\mathrm{IS}}^0$ and this introduces an unknown constant in s_c. To eliminate this ambiguity we have fixed the unknown constant for each sample by the use of (24), *i.e.* by imposing $f_{eq}(T) = \min_f \Phi(f,T)$. In all cases the correction to $s_c(f,T)$ obtained directly from (13) was found very small, giving us further confidence in the quality of our sampling. Finally we note that in this case no remarkable difference between the annealed and the quenched average has been observed.

In Figures 2 and 3 we show the complexity $s_c(f,T)$ as a function of the free energy for both the ROM and the
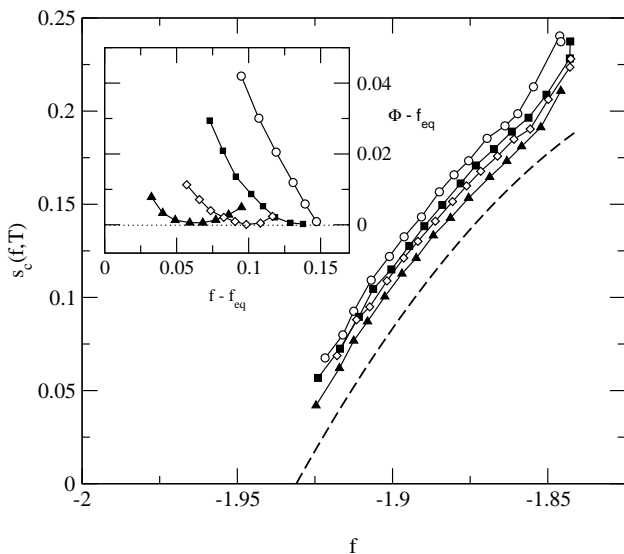
Fig. 3. Same as in Figure 2 for the ROM. Here $T = 0.8$ (circles), 0.7 (squares), 0.6 (diamonds), 0.5 (triangles), and $N = 64$. The dashed line is the analytic result [30].

SK model, compared with the corresponding $s_c(e)$, *i.e.* the $T \to 0$ limit computed analytically in references [29] and [30], respectively. In the SK model the complexity strongly depends on T. On the other hand for the ROM it is nearly T-independent and, moreover, curves at different T are remarkably parallel each other and to the zero-temperature limit, in agreement with equation (21). This behavior confirms that for the ROM the intra-valley entropy is very small, giving further justification to the results obtained in [22] using the SW decomposition.

We note that finite-size corrections are small for $s_c(f,T)$ as shown by the similarity of the results for $N = 32$ and $N = 64$. This similarity is at variance with the strong finite-size effects usually found for other quantities. For instance one finds that finite size corrections to the $P(q)$ in magnetic field in the SK model are enough strong to make the two peak structure in the glassy phase hardly visible for sizes as large as $N = 1024$ [31] (see also Ref. [32]). However one should note that we are considering probability distributions of valley dependent quantities so that finite-size effects directly affect the normalization factor in $\Phi(f,T)$ (that results in an overall constant shift in $s_c(f,T)$). This effect is further reduced by fixing the constant in the complexity self-consistently through equation (24). It seems therefore that the method could be usefully applied also to other system such as structural glasses, where $N \geq 60$ particles are known to be enough for a reasonable evaluation of s_c (for a detailed study of finite size effects in a glass forming model see Ref. [15]).

In each figure the inset shows the (averaged) shape for the potential $\Phi(f,T)$ at different temperatures. As is clearly seen the shape is different for the two models. For the SK model $\Phi(f,T)$ has a minimum $f^*(T)$ close to the lower (measured) bound over the free energy support in the whole T-range considered. The value of $f^*(T)$ con-

verges (for N large) to $f_{\mathrm{eq}}(T)$ corresponding to $s_c(f^*) = 0$. The ROM shows a different behavior. Here a local minimum appears very close to the mode-coupling transition temperature $T_{\mathrm{MCT}} = 0.6$, and moves to lower free energies as the temperature is lowered [20]. The minimum $f^*(T)$ sticks to $f_{\mathrm{eq}}(T)$ at the Kauzmann or static transition, where $s_c(f^*(T)) = 0$. From the inset of Figure 3, a simple linear extrapolation to zero of $f^*(T) - f_{\mathrm{eq}}(T)$ as function of T gives the estimate $T_K \simeq 0.26$ in excellent agreement with the theoretical value 0.25 [30].

6 Conclusions

The present FEIS approach, *i.e.* the SW decomposition based on inherent structures but considered in terms of their free energies, do capture the physics of the system even for finite T and allows for distinguish between continuous and one step RSB scenarios. It seems particularly intriguing to us that it describes well also FRSB models, where it does not correspond to a situation where time-scales are strongly separated. It moreover gives reasonable evaluations of the relevant dynamic and static transition temperatures.

In summary, we have proposed a new method to compute the configurational entropy as a function of the free energy and temperature. It provides a way to investigate the free energy landscape of glassy systems which can be generally applied whenever there is a flat measure describing the probability to dynamically explore free energy valleys. It can be used to determine the type of glassy transition (by computing the shape of the potential Φ), the mode coupling temperature and the Kauzmann temperatures.

The main advantage of method is that it allows to evaluate the complexity without using any approximation for the intra-valley entropy. Moreover, one directly obtains an evaluation of the generalized free energy Φ which contains the physics of the model. On the other hand, one should note that the method is practically limited to relative small size systems. Nevertheless, it is general enough to be applied to other models of structural glasses and spin glasses. It would be particularly interesting to consider short-range spin-glass models as well as Lennard-Jones glasses, to achieve a better understanding of the free energy landscape of generic glassy systems.

In particular in structural glasses the total number of IS is still given by (27) with α depending on the particular model and on the density, but one finds $0.7 \leq \alpha \leq 1.2$ for a Lennard-Jones model with $N = 60$ [15], which gives a very large IS number. Nevertheless it should be still possible to carry out the present kind of analysis by fixing an appropriate cutoff on p_{IS}, which simply means that one is estimating $s_c(f)$ for $f < f_{IS}^0$ instead of on the whole free energy range.

As a last remark, it is interesting to note that at variance with the present result the IS decomposition is not relevant for describing coarsening models [33], since systems sharing the same $s_c(e)$ display a different dynamical behavior.

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