Supersymmetric complexity in the Sherrington-Kirkpatrick model

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By using a supersymmetric approach we compute the complexity of the metastable states in the Sherrington-Kirkpatrick spin-glass model. We prove that the supersymmetric complexity is exactly equal to the Legendre transform of the thermodynamic free energy, thus providing a recipe to find the complexity once the free energy is known. Our results suggest that the supersymmetry may be a useful tool for the calculation of the entropy of metastable states in generic glassy systems.

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A key issue in the physics of glassy systems is the computation of the entropy of the metastable states, normally called complexity in spin glasses, and configurational entropy in structural glasses and supercooled liquids. A knowledge of the complexity is crucial for understanding the dynamics of a system when this is heavily influenced by strong metastability effects. Moreover, in some theoretical frameworks, the drop in the number of accessible states leads to an ergodicity breaking transition. In this context the complexity is essential also from the thermodynamic point of view, as in the Adam-Gibbs theory of the thermodynamic glass transition [1].

Despite its enormous theoretical relevance, there are few analytic calculations of the complexity in glassy systems, and this is for a very good reason. In a nutshell, to find the complexity we have to compute the number of local minima (metastable states) of some state function, which is typically highly nontrivial. Just to fix ideas, we may think that this function is the Hamiltonian H. To compute the complexity, we must impose that the gradient of H (the force) vanishes in the local minima, and we have to include as a normalization factor the second derivative of H (the Hessian). Moreover, we may want to classify the metastable states according to their value of H. Therefore, beside the force and the Hessian, we must include the state function itself in the calculation. Computing the complexity is thus a formidable technical task, since we have to deal with *three* very complicated functions: H, ∂H, and $\partial^2 H$. In comparison, the calculation of the partition function, which just involves H, is an easy business.

This apparent difficulty in the calculation of the complexity stems from the fact that most methods treat H, ∂H, and $\partial^2 H$ as three independent objects, when of course they are not so. Every calculation which fails to capture the fact that it is essentially just *one* function H that we are dealing with, effectively wastes a crucial information. It would be therefore important to find a tool which exploits this information to simplify the calculation of the complexity. The Becchi-Rouet-Stora-Tyutin (BRST) supersymmetry seems to be such a tool.

The BRST supersymmetry was first introduced in the context of quantum gauge theories [2,3]. Its relevance in statistical mechanics is mainly due to the fact that the generating functional associated to stochastic equations (as the Langevin equation) enjoys the BRST invariance. To build the generating functional one has to impose a δ function on the stochastic equation itself, times a normalization given by the determinant of the Jacobian of the equation. The BRST invariance is the mathematical consequence of the physical connection between the stochastic equation and its Jacobian in the generating functional [4]. Moreover, the BRST supersymmetry has been applied to the study of the random filed Ising model [5]. It was first noted in Ref. [6] that it is possible to generalize the BRST supersymmetry to the calculation of the complexity in spin glasses. it was shown for a given model that a BRST calculation of the complexity was in fact equivalent to the one of the partition function. This is indeed what we expect from a method which does *not* treat H, ∂H, and $\partial^2 H$ as independent functions.

The formal equivalence between complexity and standard thermodynamics found in Ref. [6] by means of the BRST supersymmetry is a very important theoretical issue. In the context of spin glasses the existence of such a connection has been much investigated in the past [7–15]. In a classic paper [7], Bray and Moore first calculated the complexity of the Sherrington-Kirkpatrick (SK) model [16] by counting the number of local minima of the Thouless-Anderson-Palmer (TAP) free energy [17], which in mean-field spin glasses is the state function discussed above. The same authors also noted in Ref. [8] some deep formal connections between TAP complexity and standard thermodynamics, while De Dominicis and Young showed in Ref. [10] that TAP and static approaches were in fact equivalent, once some key hypothesis were made. These studies culminated in a remarkable work [11], where Bray *et al.* uncovered a sort of Legendre transform relationship between TAP complexity and static free energy.

A method to compute the complexity which does not rely on the existence of a TAP free energy was introduced by Monasson [12] and by Franz and Parisi [13]. The basic idea is to introduce a coupling between different systems forcing them to live in the same metastable state. The free-energy cost of such a constrained supersystem is equal to the entropic contribution of the metastable states, which is the complexity. Within this approach, close connections between complexity and thermodynamics, similar to those found in the TAP context in Ref. [11], were found. In particular, in spin-glass models with one step of replica symmetry breaking (1RSB) [18], the formulation of Monasson shows that the complexity is equal to the Legendre transform of the static free energy with respect to the breaking point x of the overlap matrix [12,15].

Despite all these investigations, it is fair to say that a general formal connection between complexity of the metastable states and static free energy has not been proved yet. In particular, it is unclear how the Legendre transform method of Ref. [12] should be used in systems with more than one step of replica symmetry breaking, as in the SK model. In fact, none of the previous SK investigations [8,11] succeeded in proving the existence of a sharp Legendre transform relationship as in 1RSB systems.

In this paper we find an exact connection between complexity of the metastable states and static free energy in the SK model: we prove that the quenched TAP complexity obtained by means of the BRST supersymmetry is the Legendre transform of the static free energy with respect to the *largest* breaking point of its overlap matrix. Our result confirms the validity of the Legendre transform method of Refs. [12–14] and its consistency with the investigations of Refs. [8–11]. Moreover, our findings strongly suggest that the BRST supersymmetry should be considered as an essential tool also in more general glassy systems. For example, the analysis of the structure of the stationary points of the potential energy (both minima and saddles) in structural glasses is a very relevant issue which could benefit the supersymmetric approach.

The complexity of the TAP states with free-energy density f, at inverse temperature β, is defined as [7]

$$\Sigma(\beta,f)=\frac{1}{N}\ln\sum_{\alpha=1}^{\mathcal{N}}\delta(N\beta f-\beta F_{TAP}(m^\alpha))$$
$$=\frac{1}{N}\ln\int dr e^{Nr\beta f}\sum_{\alpha=1}^{\mathcal{N}}e^{-r\beta F_{TAP}(m^\alpha)}, \qquad (1)$$

where $m^\alpha\equiv\{m_i^\alpha\}$ are the local magnetizations at site $i=1\cdots N$ in state $\alpha=1\cdots\mathcal{N}$. A state m^α is defined as a local minimum of the TAP free energy $F_{TAP}(m)$ [17]. If we define the thermodynamic potential $\Psi(\beta,r)$,

$$\exp(-\beta Nr\Psi)\equiv\sum_{\alpha=1}^{\mathcal{N}}e^{-r\beta F_{TAP}(m^\alpha)}, \qquad (2)$$

we can use the steepest descent method in Eq. (1) and obtain the complexity as the Legendre transform of $\Psi(\beta,r)$,

$$\Sigma(\beta,f)=\beta rf-\beta r\Psi(\beta,r), \qquad (3)$$

where the parameter $r=r(\beta,f)$ is fixed by the equation

$$\Psi(\beta,r)+r\frac{\partial\Psi(\beta,r)}{\partial r}=f. \qquad (4)$$

From Eq. (2) we see that for $r=1$ the potential Ψ must be equal to the standard static free energy of the system $F(\beta)$, calculated in the TAP context. This calculation was first performed in Ref. [10], where it was shown that the relation $\Psi(\beta,r=1)=F(\beta)$ only held if some suitable assumptions were made. In Ref. [19] it was proved that the assumptions used in Ref. [10] were in fact a general consequence of the BRST supersymmetry. In what follows we perform a supersymmetric quenched calculation of $\Psi(\beta,r)$ for generic r. The TAP free energy for the SK model is given by [17]

$$\beta F_{TAP}(m)=-\frac{\beta}{2}\sum_{ij}J_{ij}m_im_j+\frac{1}{\beta}\sum_i\phi_0(m_i), \qquad (5)$$

$$\phi_0(m)=\frac{1}{2}\ln(1-m^2)+m\tanh^{-1}(m)-\ln 2-\frac{\beta^2}{4}(1-q)^2. \qquad (6)$$

The variable q is the self-overlap of the TAP states, $q=1/N\Sigma_im_i^2$. The quenched couplings J are random variables with Gaussian distribution and variance N. From Eq. (2) we have that the *quenched* potential $\Psi(\beta,r)$ is

$$-\beta r\Psi(\beta,r)=\frac{1}{nN}\ln\overline{\rho(\beta,r|J)^n}, \qquad (7)$$

$$\rho(\beta,r|J)=\sum_{\alpha=1}^{\mathcal{N}}e^{-r\beta F_{TAP}(m^\alpha)}$$
$$=\int\prod_i dm_i\delta(\partial_iF_{TAP}(m))$$
$$\times|\det(\partial_i\partial_jF_{TAP}(m))|e^{-\beta rF_{TAP}(m)}. \qquad (8)$$

In Eq. (7) we have $N\to\infty$ and $n\to 0$, and the over-bar indicates an average over the disorder. As usual, the modulus of the determinant will be dropped. This amounts to assuming that at sufficiently low temperatures the largest part of TAP solutions are minima. Of course, any method which drops the modulus is doomed to fail if stable minima are subdominant with respect to unstable saddles. After introducing the commuting fields x_i to implement the δ functions and the anticommuting (Grassmann) fields $\overline{\psi}_i,\psi_i$ for the determinant, we find

$$\rho(\beta,r|J)=\int\mathcal{D}m\mathcal{D}x\mathcal{D}\overline{\psi}\mathcal{D}\psi e^{\beta S(m,x,\overline{\psi},\psi)}, \qquad (9)$$

where the action S is given by

$$S(m,x,\overline{\psi},\psi)=\sum_i x_i\partial_iF_{TAP}(m)+\sum_{ij}\overline{\psi}_i\psi_j\partial_i\partial_jF_{TAP}(m)$$
$$-rF_{TAP}(m). \qquad (10)$$

Before substituting the actual form of the TAP free energy in the equation above, it is useful to consider the role of the supersymmetry. Indeed, as first noted in Ref. [6], action (10) is invariant under the following generalization of the BRST transformation [2,3],

$$\delta m_i=\epsilon\psi_i, \qquad \delta x_i=\epsilon r\psi_i, \qquad \delta\overline{\psi}_i=-\epsilon x_i, \qquad \delta\psi_i=0, \qquad (11)$$

where ϵ is an infinitesimal Grassmann parameter. If we average the variation of $m_i \cdot \overline{\psi_i}$ and of $x_i \cdot \overline{\psi_i}$ [6,19], we obtain the two Ward identities associated to the BRST supersymmetry,

$$\langle \overline{\psi_i}\psi_i\rangle + \langle m_i x_i\rangle = 0, \tag{12}$$

$$r\langle \overline{\psi_i}\psi_i\rangle + \langle x_i x_i\rangle = 0. \tag{13}$$

We note that the supersymmetric form of action (10) and the validity of BRST relations (12) and (13) are completely general, since they do not depend on the explicit form of the function whose stationary point are considered. In the present case this function is the TAP free energy, but in another model it could equally be the potential energy, or any other function of the local degrees of freedom.

To average $\rho(\beta,r|J)^n$ over the disorder we introduce replicas and the scalar overlap q will now be generalized by introducing the overlap matrix $q_{ab} = m^a \cdot m^b$. In order to linearize the quadratic terms generated by the average over the disorder we introduce the usual Lagrange multipliers [19], $m^a m^b \to \lambda_{ab}$, $m^a x^b \to w_{ab}$, $\overline{\psi}^a \psi^b \to t_{ab}$. After this is done, the integrals in x and $\overline{\psi},\psi$ become Gaussian and can be performed explicitly. Moreover, the action factorizes and for $N \to \infty$ we can use the steepest descent method to get

$$-\beta r \Psi(\beta,r) = \lim_{n\to 0} \frac{1}{n}\left[\Sigma_0 + \ln \int \prod_a dm^a e^{\mathcal{L}(m^a)}\right]. \tag{14}$$

Following Refs. [7,9,19] we define

$$B_{ab} \equiv \beta^2 (1-q_{aa})\delta_{ab} + t^{ab}, \tag{15}$$

$$\Delta_{ab} \equiv -\beta^2 (1-q_{aa})\delta_{ab} - w^{ab}, \tag{16}$$

and therefore obtain (see Ref. [22] for details)

$$\Sigma_0 = \frac{1}{2\beta^2}\sum_{ab} (B_{ab}^2 - \Delta_{ab}^2) - \sum_a (B_{aa}+\Delta_{aa})(1-q_{aa}) - \sum_{ab}\left[\frac{\beta^2}{4} r^2 q_{ab}^2 + \lambda^{ab} q_{ab} - r\Delta^{ab} q_{ab}\right] - \frac{1}{2}\ln[(2\pi\beta^2)^n \det q_{ab}], \tag{17}$$

$$\mathcal{L}(m^a) = -r\sum_a \phi_0(q_{aa},m^a) + \sum_{ab} \lambda^{ab} m^a m^b + \ln\det\left(\frac{\delta_{ab}}{1-m_a^2} + B_{ab}\right) - \frac{1}{2\beta^2}\sum_{ab}\left[\tanh^{-1} m^a - \sum_c \Delta^{ac} m^c\right] q_{ab}^{-1}\left[\tanh^{-1} m^b - \sum_c \Delta^{bc} m^c\right]. \tag{18}$$

The parameters Δ_{ab}, B_{ab}, λ_{ab}, and q_{ab} must be fixed by the saddle point equations and it is easy to show that $B_{ab} = 0$ is solution [7,11,19].

It is important to note that the supersymmetric transformations on the original parameters (11) propagate to the new variational parameters in Eqs. (17) and (18). In this way the BRST Ward identities (12) and (13) give rise to the two following extra relations for the variational parameters:

$$\Delta_{ab} = \beta^2 q_{ab} r, \tag{19}$$

$$\lambda_{ab} = \frac{1}{2}\beta^2 r^2 q_{ab}. \tag{20}$$

These two identities select among the (potentially many) solutions of the saddle point equations, the BRST supersymmetric one. At the annealed level, in addition to the BRST solution discussed in Ref. [19], there is also a non-BRST one, discovered in Ref. [7], and they have quite different properties. Even though the annealed BRST solution reproduces the static results at the 1RSB level, it is still an open issue whether or not this is indeed the correct solution at the annealed level [20,21]. However, in order to have physically relevant results at *low* free energies, the quenched calculation is required, and we do not know at the moment whether it exists, and what is the form of a quenched *non*-BRST solution of the saddle point equations, since the previous quenched calculation of Ref. [11] has been proved to be in fact a supersymmetric one [21,22]. On the other hand, the BRST solution we present here does reproduce the correct static results at the quenched level, providing, for example, the correct equilibrium free energy at the lower band edge, and a direct connection with the static free-energy functional.

Once the BRST identities are imposed, the only saddle point equation we are left with is obtained by doing the variations of Eq. (17) and (18) with respect to λ_{ab}. This gives the relation $q_{ab} = \langle\langle m^a m^b\rangle\rangle$, where the average is performed with the distribution $\exp(\mathcal{L}(m^a))$. If we use Eqs. (19) and (20) into Eqs. (17) and (18), and make the change of variable $m^a \to h^a = \tanh^{-1}(m^a)$, we finally obtain

$$\beta\Psi(\beta,r) = -\ln 2 + \frac{\beta^2}{4n}\left[r\sum_{ab}^{n} q_{ab}^2 - \sum_a^n (1-q_{aa})^2\right] - \frac{1}{nr}\ln\int\prod_a^n \frac{dh^a}{\sqrt{2\pi\beta^2 \det q_{ab}}}\cosh(h^a)^r \times \exp\left(-\frac{1}{2\beta^2}\sum_{ab}^n h^a q_{ab}^{-1} h^b\right). \tag{21}$$

The BRST supersymmetry has drastically reduced the number of parameters, and the computation of $\Psi(\beta,r)$ has at this point the same degree of complication as that of the standard free energy $F(\beta)$, with just one overlap matrix q_{ab} to be fixed variationally. We shall now show that the connections between $\Psi(\beta,r)$ and $F(\beta)$ are in fact much deeper than that. The general form of the SK quenched free energy in terms of replicated spins is [16]

$$\beta F(\beta) = -\frac{\beta^2}{4} + \frac{\beta^2}{2n_s} \sum_{\alpha>\beta}^{n_s} Q_{\alpha\beta}^2 - \frac{1}{n_s} \ln \sum_{[\sigma^\alpha=\pm 1]} \exp\left[\frac{\beta^2}{2} \sum_{\alpha\neq\beta}^{n_s} Q_{\alpha\beta}\sigma^\alpha\sigma^\beta\right], \tag{22}$$

where the σ^α are the replicated spin variables with $\alpha = 1,\dots,n_s$ and $Q_{\alpha\beta}$ is the $n_s\times n_s$ overlap matrix, with $n_s \to 0$. By introducing in Eq. (21) the auxiliary spin variables τ_a^μ, with $a=1,\dots,n$ and $\mu=1,\dots,r$, we can rewrite $\Psi(\beta,r)$ as

$$\beta\Psi(\beta,r) = -\frac{\beta^2}{4} + \frac{\beta^2}{2n}\left[r\sum_{a>b}^{n} q_{ab}^2 + \frac{r-1}{2}\sum_{a}^{n} q_{aa}^2\right] - \frac{1}{nr}\ln\sum_{[\tau_a^\mu]} \exp\left[\frac{\beta^2}{2}\left(\sum_{ab}^{n}\sum_{\mu\nu}^{r} \tau_a^\mu q_{ab}\tau_b^\nu - \sum_{a}^{n}\sum_{\mu}^{r} q_{aa}\right)\right]. \tag{23}$$

A comparison of the two trace terms in Eqs. (22) and (23) suggests the relation $n_s = rn$. Once this identification is done, we can connect the σ^α spin variables, to the τ_a^μ spin variables in the following way:

$$(\sigma_1,\dots,\sigma_{n_s}) = (\tau_1^1,\dots,\tau_1^r,\dots\ \dots,\tau_n^1,\dots,\tau_n^r).$$

Let us now assume that the potential $\Psi(\beta,r)$ (and thus the TAP complexity) is calculated at k levels of RSB [18]. The TAP overlap matrix q_{ab} is then given by

$$q_{ab}^{(k)} = q_0 + \sum_{i=1}^{k+1} (q_i - q_{i-1})\varepsilon_{ab}^{(n,y_i)}, \tag{24}$$

with $y_{k+1}=1$. The matrices $\varepsilon^{(n,y_i)}$ are $n\times n$ ultrametric block matrices, equal to one on the diagonal blocks of size y_i, and zero elsewhere ($\varepsilon_{ab}^{(n,1)} = \delta_{ab}$). The variables y_i are thus the replica symmetry breaking points. In the TAP approach the diagonal of the overlap matrix, $q_{aa} = q_{k+1}$, contains the self-overlap of the states, and for this reason $y_{k+1} = 1$. There are $k+1$ values of the overlap, but only k nontrivial breaking points, and thus q_{ab} is a k RSB matrix. Given this form of q_{ab}, it is possible to prove that [22]

$$\sum_{ab}^{n}\sum_{\mu\nu}^{r} \tau_a^\mu q_{ab}^{(k)}\tau_b^\nu - \sum_{a}^{n}\sum_{\mu}^{r} q_{aa}^{(k)} = \sum_{\alpha\neq\beta}^{rn} Q_{\alpha\beta}^{(k+1)}\sigma_\alpha\sigma_\beta, \tag{25}$$

where $Q_{\alpha\beta}^{(k+1)}$ is a standard $rn\times rn$ RSB matrix, with $k+1$ levels of replica symmetry breaking. More precisely,

$$Q_{\alpha\beta}^{(k+1)} = q_0 + \sum_{i=1}^{k+1} (q_i - q_{i-1})\varepsilon_{\alpha\beta}^{(rn,ry_i)}. \tag{26}$$

From this formula we see that the entries of $Q_{\alpha\beta}^{(k+1)}$ are the same as $q_{ab}^{(k)}$, whereas the $k+1$ replica symmetry breaking points x_i of $Q_{\alpha\beta}^{(k+1)}$ are rescaled by a factor of r, that is, $x_i = r\,y_i$. In particular, the *largest* breaking point x of the static matrix $Q_{\alpha\beta}^{(k+1)}$ is given by $x \equiv x_{k+1} = r$. By inserting relation (25) into (23), we finally obtain

$$\Psi(\beta,r|q_{ab}^{(k)}) = F(\beta|Q_{ab}^{(k+1)}). \tag{27}$$

We have thus proved that the thermodynamic potential $\Psi(\beta,r)$ calculated at the k-RSB level is equal to static free energy $F(\beta)$ calculated at the $k+1$ RSB level. The replica symmetry breaking points of the static matrix $Q_{\alpha\beta}$ are simply the ones of the TAP matrix q_{ab} rescaled by the parameter r, and the extra $(k+1)$th breaking point of $Q_{\alpha\beta}$ is equal to r. This rescaling was first noted in Ref. [11], and later in Ref. [14], although the lack of BRST symmetry of those calculations prevented to prove Eq. (27).

From Eq. (3), and given the relation between $\Psi(\beta,r)$ and $F(\beta)$, we finally have the general Legendre equation connecting the quenched complexity of the TAP states to the standard static free energy in the SK model,

$$\Sigma(\beta,f) = \beta x f - \beta x F(\beta;x), \tag{28}$$

with the largest breaking point x fixed by the equation

$$f = F(\beta;x) + x\frac{\partial F(\beta;x)}{\partial x}. \tag{29}$$

This result can be summarized as follows: *the supersymmetric quenched complexity of the TAP states is the Legendre transform of the static free energy with respect to the largest breaking point x* of its overlap matrix.

It has been conjectured in Ref. [23] that in systems with more than one step of replica symmetry breaking the complexity of *clusters* at level i is given by the Legendre transform of the free energy with respect to the breaking point x_i. For $x_i = x_{max}$ clusters are just states, and our result is recovered. It would be interesting to study whether the conjecture of Ref. [23] can be exactly proved within the supersymmetric formalism used here.

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