Adv. Studies Theor. Phys., Vol. 1, 2007, no. 1, 29 - 37

Free Energy Expansion in Quasi Stationary ROSt

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Abstract

In this paper we derive recursively an expression for the free energy of the Sherrington-Kirkpatrick (SK) model in the framework of Random Overlap Structures (ROSt) recently introduced by Aizenman and coworkers. This expression is obtained in the optimal Boltzmann ROSt via the infinite irreducible overlap correlation functions, which act globally as a sort of order parameter of the theory. In the very promising ROSt approach to spin glasses it turns out that the Derrira-Ruelle GREM acts an optimal ROSt and, in a sense, it contains Parisi theory in itself. On the other side Guerra showed that the Boltzmann ROSt shares the optimality property too, raising the interest for a comparison between these structures, to understand if they can be the same or they lead to the same free energy but are different (i.e. in the organization of the pure states in the low temperature regime). We find that our expression is exactly the expansion obtained in the standard cavity field approach for the SK model. As it has been already proven, Aizenman-Contucci relations hold in the Boltzmann ROSt, and along the same lines stemming from stochastic stability we show here that this ROSt enjoys many features of the solution obtained via replica analysis. We also show how the extension to all the quasi-stationary (generally optimal) ROSt's is conceived.

Keywords: Spin Glasses, Random Overlap Structures, Quasi-Stationarity

1 Introduction

From its early days, statistical mechanics of spin glasses has been very challenging from both the physical and the mathematical point of view. It took several years since the main model (the Sherrington-Kirkpatrick, or simply SK) was introduced to compute the free energy, through the ingenious intuition of Parisi, i.e. his choice of replica symmetry breaking (see [11] and references therein). It took even longer to obtain a fully rigorous proof of Parisi formula [10, 12]. Recently, Aizenmann, Sims and Starr [1] introduced another approach, based on their Random Overlap Structures (henceforth ROSt). This approach is the proper way to implement the cavity method. Within this framework Parisi theory comes in the GREM formulation of Derrida-Ruelle [4, 5] and it turns out to be an extremal for the ROSt variational principle. On the other hand, in [9], Guerra showed that the structures that yield the exact value of the free energy (the optimal structures) must fulfill certain constraints and these structures will be called Boltzmann ROSt hereafter . In [7] it has been shown that in these optimal structures (Boltzmann ROSt) the Aizenman-Contucci (AC) constraints hold too. AC polynomials are constraints on the distribution of the overlaps, and were known to be a consequence of stochastic stability, in full agreement with Parisi theory. So a first step in the comparison between these two optimal ROSt has been achieved. In this paper we perform an expansion the free energy of the SK model within the Boltzmann ROSt, and find that it is the same expansion obtained within the usual cavity method [6] again in agreement with Parisi theory.

The paper is organized as follows. In section 2 we introduce the SK model and the concept of ROSt to state the Extended Variational Principle [1]. In section 3 we present the main results regarding the expansion of the free energy in the Boltzmann ROSt. In section 4 we emphasize that the same results are valid in any Quasi-Stationary ROSt, leaving section 5 for conclusions and remarks.

2 Model and notations

The SK model describes a system of N binary spins $\sigma_i, i \in \{1, \dots, N\}$. A configuration σ of the system is then a map

$$\sigma : \{1, 2, ..., N\} \ni i \to \sigma_i \in \{-1, +1\} \ .$$

The Hamiltonian of the model is defined to assign the following energy to a given configuration σ:

$$H_N(\sigma; J) = -\frac{1}{\sqrt{N}} \sum_{(i,j)}^{1,N} J_{ij}\sigma_i\sigma_j \ ,$$

where the sum ranges over all the $N(N-1)/2$ different couples of indices (i,j), and J_{ij} are independ centered unit Gaussian random variables. The partition function is defined as usual by

$$Z_N(\beta;J) = \sum_\sigma \exp(-\beta H(\sigma;J)) \ ,$$

while the Boltzmann-Gibbs expectation of an observable $A:\sigma \to \mathbb{R}$ is

$$\omega(A) = \frac{1}{Z_N(\beta;J)} \sum_\sigma A(\sigma) \exp(-\beta H(\beta;J)) \ . \tag{1}$$

The global average (over the thermal bath first and the noise in the coupling then) is $\langle\cdot\rangle = \mathbb{E}\omega(\cdot)$, where $\mathbb{E}$ denotes the expectation with respect to all the (quenched) Gaussian variables.

By Ω we denote the product measure (*replica measure*) of the needed number of copies of ω, which we will use when dealing with functions of several configurations (replicas). Notice that while Ω is factorized by definition, $\langle\cdot\rangle$ is not, as we are just replicating configurations keeping for each the same disorder (i.e. Gaussian couplings). Taking the same disorder results in coupling the various replicas and therefore $\mathbb{E}$ destroys the factorization. Given two replicas $\sigma^{(1)}$ and $\sigma^{(2)}$ we define the overlap between them as

$$q_{12} = \frac{1}{N} \sum_{i=1}^N \sigma_i^{(1)} \sigma_i^{(2)} \ .$$

The pressure $\alpha_N(\beta)$ and the free energy per spin $f_N(\beta)$ are defined as

$$\alpha_N(\beta) = -\beta f_N(\beta) = \frac{1}{N} \mathbb{E} \ln Z_N(\beta) \ . \tag{2}$$

Let us now introduce an auxiliary system.

Definition 1 *A* Random Overlap Structure $\mathcal{R}$ *is a triple* $(\Sigma, \tilde{q}, \xi)$ *where*

- $\Sigma \ni \gamma$ *is a discrete space;*
- $\xi : \Sigma \to \mathbb{R}_+$ *is a system of random weights, such that* $\sum_{\gamma\in\Sigma} \xi_\gamma < \infty$*;*
- $\tilde{q} : \Sigma^2 \to [0,1], |\tilde{q}| \leq 1$ *is a positive definite* Overlap Kernel *(equal to 1 only on the diagonal of* Σ^2*).*

The randomness in the weights ξ is independent of the randomness of the quenched variables from the original system with spins σ. We equip a ROSt with two families of independent and centered Gaussians $\tilde{h}_i$ and $\hat{H}$ with covariances

$$
\begin{aligned}
\mathbb{E}[\tilde{h}_i(\gamma)\tilde{h}_j(\gamma')] &= \delta_{ij}\tilde{q}_{\gamma\gamma'} \ , && (3)\\
\mathbb{E}[\hat{H}(\gamma)\hat{H}(\gamma')] &= \tilde{q}^2_{\gamma\gamma'} \ . && (4)
\end{aligned}
$$

Given a ROSt $\mathcal{R}$ we define the trial pressure as

$$
G_N(\mathcal{R}) = \frac{1}{N}\mathbb{E}\ln\frac{\sum_{\sigma,\gamma}\xi_\gamma\exp(-\beta\sum_{i=1}^N\tilde{h}_i(\gamma)\sigma_i)}{\sum_\gamma\xi_\gamma\exp(-\beta\sqrt{\frac{N}{2}}\hat{H}(\gamma))} \ . \tag{5}
$$

The following theorem [1] can be easily proven by interpolation

Theorem 1 (Extended Variational Principle) *Infimizing for each N separately the trial function $G_N(\mathcal{R})$ defined in (5) over the whole ROSt space, the resulting sequence tends to the limiting pressure $-\beta f(\beta)$ of the SK model as N tends to infinity*

$$
\alpha(\beta) = \lim_{N\to\infty}\alpha_N(\beta) = \lim_{N\to\infty}\inf_{\mathcal{R}} G_N(\mathcal{R}) \ .
$$

A ROSt $\mathcal{R}$ is said to be optimal if $\lim_{N\to\infty} G_N(\mathcal{R}) = \alpha$ for any inverse temperature β. An optimal ROSt is the so-called Boltzmann ROSt $\mathcal{R}_B$, defined as follows. Take $\Sigma = \{-1, 1\}^M$, and denote by τ the points of Σ. We clearly have in mind an auxiliary spin system (and that is why we use τ as opposed to the previous γ to denote its points). In fact, we also choose

$$
\tilde{h}_i = -\frac{1}{\sqrt{M}}\sum_{k=1}^M\tilde{J}_{ik}\tau_k \ , \quad \hat{H} = -\frac{1}{M}\sum_{k,l}^{1,M}\hat{J}_{kl}\tau_k\tau_l
$$

which satisfy (3)-(4) with $\tilde{q}_{\tau\tau'} = \frac{1}{M}\sum_k\tau_k\tau'_k$, and $\tilde{J}$ and $\hat{J}$ are families of i.i.d. random variables independent of the original couplings J, with whom they share the same distribution. The variables $\tilde{h}_\cdot$ are called *cavity fields*. Let us also choose

$$
\xi_\tau = \exp(-\beta H_M(\tau)) \ .
$$

If we call $\mathcal{R}_B(M)$ the structure defined above, we will formally write $\mathcal{R}_B(M) \to \mathcal{R}_B$ as $M \to \infty$, and we call $\mathcal{R}_B$ the Boltzmann ROSt. The reason why such a ROSt is optimal is purely thermodynamical, and equivalent to the existence of the thermodynamic limit of the free energy per spin. A detailed proof of this fact can be found in [1]; here we just mention the main point:

$$
\alpha(\beta) = \lim_{N\to\infty}\mathbf{C}\lim_M G_N(\mathcal{R}_B(M)) = G_N(\mathcal{R}_B) = G(\mathcal{R}_B)
$$

where $\mathbf{C}\lim$ is the limit in the Cesàro sense. Notice that the Boltzmann ROSt does not depend on N, after the M-limit.

3 Free energy expansion in $\mathcal{R}_B$

The expression we want to consider for the expansion is:

$$\alpha(\beta) = \frac{1}{N}\mathbb{E}\ln\Omega(2^N\prod_i^N \cosh(\beta\tilde{h}_i)) - \frac{1}{N}\mathbb{E}\ln\Omega\Big(\exp\Big(-\beta\sqrt{\frac{N}{2}}\hat{H}\Big)\Big) \tag{6}$$

which is the trial pressure $G(\mathcal{R}_B)$, defined in (5), computed at the (optimal) Boltzmann ROSt $\mathcal{R}_B$, defined in the previous section.

Let us start from the first term in the right hand side of (6). If we define

$$c_i = 2\cosh(\beta\tilde{h}_i) = \sum_{\sigma_i}\exp(-\beta\tilde{h}_i\sigma_i)\ ,$$

then

$$\frac{1}{N}\mathbb{E}\ln\Omega\sum_\sigma \exp(-\beta\sum_{i=1}^N \tilde{h}_i\sigma_i) = \frac{1}{N}\mathbb{E}\ln\Omega(c_1\cdots c_N) \tag{7}$$

does not depend on N [9, 8], if we consider the infinite Boltzmann ROSt, where $M\to\infty$. Assume we replace the β in front of the cavity fields $\tilde{h}_.$ (but not in the state Ω) with a parameter $\sqrt{t}$, and define, upon rescaling,

$$\Psi(t) = \mathbb{E}\ln\Omega\sum_\sigma \exp\frac{\sqrt{t}}{\sqrt{N}}\sum_{i=1}^N \tilde{h}_i\sigma_i\ . \tag{8}$$

We want to study the flux (in t) of equation (8), to obtain for it an integrable expansion. Notice that obviously

$$\frac{1}{N}\mathbb{E}\ln\Omega(2^N\prod_i^N\cosh(\beta\tilde{h}_i)) = \frac{1}{N}\lim_{t\to N\beta^2}\Psi(t)\ .$$

The t-flux of the cavity function Ψ is given by

$$\partial_t\Psi(t) = \frac{1}{2}(1-\langle q_{12}\tilde{q}_{12}\rangle_t)\ , \tag{9}$$

which is easily seen by means of a standard use of Gaussian integration by parts. The subscript in $\langle\cdot\rangle_t = \mathbb{E}\Omega_t$ means that such an average includes in the Boltzmannfaktor the t-dependent exponential appearing in (8). Now the way to proceed is simple: we have to expand the t-derivative of $\Psi(t)$ until a closed-form expression is obtained, then we can give place to an order by order expansion of the (modified) denominator of the Boltzmann ROSt (that is the first term of (6), i.e. the function $N^{-1}\psi(t)$ evaluated at $t = N\beta^2$). So we are expanding in powers of t (or equivalently in powers of the overlap $\tilde{q}$, because there is a one to one correspondence between powers of t or β^2 and powers of $\tilde{q}$; in fact, in what follows we will refer to the fifth order thinking of $\tilde{q}^5$ or β^{10}).

The techniques employed in the expansion are illustrated in [7] and [6], so here we skip the long but straightforward iteration, and proceed with the extension of the results of [7] to our case. We are hence about to exhibit the fifth one, which is known to play a crucial role in the theory of replica symmetry breaking.

The cavity fields in 8 clearly act paramegnetically on the spins, the sum over which can therefore easily be performed explicitly. So proceeding we obtain expressions for the q-overlap correlation functions, and namely, the ones we find at the fifth order are:

$$\begin{aligned}
\langle q_{12}^2 q_{34} q_{45} q_{35} \rangle &= \frac{\mathbb{E}}{N^5} \sum_{ijklm} \omega(\sigma_i\sigma_j)\omega(\sigma_j\sigma_k)\omega(\sigma_i\sigma_k)\omega^2(\sigma_l\sigma_m) = \frac{1}{N^3}, \\
\langle q_{12}^2 q_{23} q_{34} q_{24} \rangle &= \frac{\mathbb{E}}{N^5} \sum_{ijklm} \omega(\sigma_i\sigma_j\sigma_k\sigma_l)\omega(\sigma_i\sigma_j)\omega(\sigma_k\sigma_m)\omega(\sigma_m\sigma_l) = \frac{1}{N^3}, \\
\langle q_{12} q_{23} q_{34} q_{45} q_{15} \rangle &= \frac{\mathbb{E}}{N^5} \sum_{ijklm} \omega(\sigma_i\sigma_j)\omega(\sigma_j\sigma_k)\omega(\sigma_k\sigma_l)\omega(\sigma_l\sigma_m)\omega(\sigma_m\sigma_i) = \frac{1}{N^4}, \\
\langle q_{12}^3 q_{23} q_{13} \rangle &= \frac{\mathbb{E}}{N^5} \sum_{ijklm} \omega(\sigma_i\sigma_j\sigma_k\sigma_l)\omega(\sigma_i\sigma_j\sigma_k\sigma_l)\omega(\sigma_l\sigma_k) = \frac{1+3(N-1)}{N^4}.
\end{aligned}$$

From now on, as the q-overlaps have been calculated explicitly, we can use a graphical formalism [6, 7]: we use points to identify replicas and lines for the overlaps between them. So for example:

$$\langle \bullet\!\!-\!\!\bullet \rangle = \langle \tilde{q}_{12} \rangle, \qquad \langle \bigcirc \rangle = \langle \tilde{q}_{12}^2 \rangle, \qquad \langle \triangle \rangle = \langle \tilde{q}_{12}\tilde{q}_{23}\tilde{q}_{13} \rangle$$

and so on. We have thus from (7)-(8)

$$\frac{\mathbb{E}}{N} \ln \Omega(2^N \prod_i^N \cosh(\beta \tilde{h}_i)) = \frac{1}{2} \lim_{t\to\beta^2} \int_0^t [1 - \langle q_{12}\tilde{q}_{12} \rangle_{t'}] dt' \ .$$

Therefore proceeding like in [7] we have the expansion at the fifth order of (6)

$$\begin{aligned}
\frac{\Psi(\beta^2 N)}{N} = \frac{\beta^2}{2} - \langle \bigcirc \rangle \frac{\beta^4}{4} + \langle \triangle \rangle \frac{\beta^6}{3} + \langle \bigcirc\!\bigcirc \rangle \frac{\beta^8}{6} - \langle \substack{\bigcirc \\ \bigcirc} \rangle \frac{\beta^8}{8} - \langle \square \rangle \frac{3\beta^8}{4} \\
- \beta^{10} \langle \bigcirc\!\!\lhd \rangle + \frac{12\beta^{10}}{5} \langle \pentagon \rangle + \langle \bigcirc\!\!\lhd \rangle \frac{2\beta^{10}}{3} - O(\beta^{12}) \ .
\end{aligned}$$

Let us now focus on the second term of the trial pressure $G(\mathcal{R}_B)$, computed at the Boltzmann ROSt, defined in the previous section. Let us normalize this quantity by dividing by Z_N and let us weight $\hat{H}$ with an independent variable β', as opposed to β appearing in ω. The following equation has been proven in [7]:

$$\frac{1}{N}\mathbb{E}\ln\Omega\exp\left(-\beta'\sqrt{\frac{N}{2}}\hat{H}(\tau)\right) = \frac{\beta'^2}{4}(1-\langle\ \rangle)\ . \tag{10}$$

Putting together both the results we get:

Proposition 1 *The free energy expansion of the Boltzmann Random Overlap Structure is:*

$$\alpha(\beta) = \ln 2 + \frac{\beta^2}{4}[1+(1-\beta^2)\langle\ \rangle] + \frac{\beta^6}{3}\langle\ \rangle + \frac{\beta^8}{6}\langle\ \rangle -$$
$$\frac{\beta^8}{8}\langle\ \rangle - \frac{3\beta^8}{4}\langle\ \rangle - \beta^{10}\langle\ \rangle + \frac{12\beta^{10}}{5}\langle\ \rangle + \frac{2\beta^{10}}{3}\rangle\ \rangle + O(\beta^{12}).$$

Iterating the method we can have the pressure expansion (and obviously the free energy expansion following eq.(5)) at every desired order in the Boltzmann ROSt. It is very important to notice that, at least at these first orders computed here, the expansio is the same we obtained in [6], where it was obtained outside the framework of the Random Overlap Structures and of the Borken Replica Symmetry ansatz [11].

4 Extension to all Quasi-Stationary ROSt's

For sake of simplicity, all the explicit calculation we performed took into account the Boltzmann structure only. But the whole content actually does not depend on the explicit form of the Hamiltonians, it merely relies on the Gaussian nature of the random variables and their moments, independently of the space they are defined in. In other words, as long as we consider centered Gaussian variables, the whole treatment depends only on their covariances. That is why changing the ROSt does not change the results, except the overlaps in the various expressions will be those of the considered ROSt (e.g. the ultrametric Parisi trial overlaps), provided some properties are preserved (Quasi-Stationarity). See [3, 9] for details.

Let us focus for instance on the internal energy part, which is simpler, and notice that the stochastic stability in (10) is preserved in any Quasi-Stationary ROSt. Our proofs never makes use of the explicit form of the Hamiltonians but are determined purely by the covariances of these Hamiltonians. So the validity of the results coincides with the validity of Lemma 10. The ROSt's for which such a lemma holds are called Quasi-Stationary (see [3, 5, 9]), in this case with respect to the Cavity Step (see [9, 3]). The entropy part is fully analogous, thanks to [9]. Notice that the left hand side of (10) is zero for $\beta' = 0$ independently of the particular ROSt. Hence by the fundamental theorem of calculus the same left hand side coincides with the integral from zero to β' of its derivative (with respect to β'). But the form of such a derivative is just determined by the covariance of $\hat{H}$ (this is at the heart of [1]), which is always defined to be an overlap. Therefore a simple Gaussian integration by parts, as illustrated in [1], leads to the right hand side of (10). These are the intuitive reasons that heuristically explain why our expansion is the same in any Quasi-Stationary ROSt, no matter what the overlap looks like in a generic abstract space. Surely if the chosen ROSt is Quasi-Stationary, but not optimal, there will be no overlap locking and the trial overlap will have very little to share with the true ones of the model. Moreover (10) will not in general provide the internal energy of the model (but this can be the case in some optimal ROSt's too, like the Parisi one).

5 Conclusions and Outlook

In the paper we shown how to expand via all the overlap correlation functions the free energy of the Boltzmann (and all the quasi-stationary) ROSt as an alternative approach in the understanding thermodynamics of the SK model. Not surprisingly our expansion coincide with the expansion of the SK model itself obtained in the cavity field framework.
Restricting to the SK, after the main development of the ROSt [1], a first step further has been taken in [9] where some invariance of these structures have been obtained and in [7] where some restriction to the free overlap fluctuation have been proved. Our present result can be considered as another step on the same line in their investigation. A further step should bring the Ghirlanda-Guerra identities, and then hopefully a proof of ultrametricity.

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Received: January 11, 2007