

Exact Solutions for Diluted Spin Glasses and Optimization Problems

Silvio Franz,¹ Michele Leone,^{1,2} Federico Ricci-Tersenghi,¹ and Riccardo Zecchina¹

¹*ICTP, Condensed Matter Group, P.O. Box 586, I-34014 Trieste, Italy*

²*SISSA, Via Beirut 9, I-34014 Trieste, Italy*

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We study the low temperature properties of p -spin glass models with finite connectivity and of some optimization problems. Using a one-step functional replica symmetry breaking ansatz we can solve exactly the saddle-point equations for graphs with uniform connectivity. The resulting ground state energy is in perfect agreement with numerical simulations. For fluctuating connectivity graphs, the same ansatz can be used in a variational way: For p -spin models (known as p -XOR-SAT in computer science) it provides the exact configurational entropy together with the dynamical and static critical connectivities (for $p = 3$, $\gamma_d = 0.818$, and $\gamma_s = 0.918$), whereas for hard optimization problems like 3-SAT or Bicoloring it provides new upper bounds for their critical thresholds ($\gamma_c^{\text{var}} = 4.396$ and $\gamma_c^{\text{var}} = 2.149$).

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The nature of the glassy phase and of the out-of-equilibrium dynamics of physical systems are two intertwined aspects of the behavior of many complex systems found in different fields, ranging from physics or biology to computer science and game theory. The existence and the characterization of long time states and the question of relaxation times are important open issues of modern statistical mechanics and probability theory.

Fully connected spin glasses have served as prototype models able to provide a highly nontrivial static and off-equilibrium phenomenology already at the mean-field level [1,2]. However, some important features of complex real-world systems heavily rely on the connectivity pattern which is particularly simple in these systems.

For instance, supercooled liquids and structural glasses are characterized by a finite number of short range interactions for each particle (bounded by the so-called *kissing number* of the particles), which leads to a complex structure of energy and entropy barriers in phase space. Heterogeneities in both the static and the off-equilibrium regimes witness such underlying constraints [3].

In computer science, nontrivial ensembles of hard combinatorial optimization problems, the so-called NP-complete problems [4], typically map onto spin glasses with finite average connectivity (or degree) at zero temperature [5]. In the last years methods from statistical physics have been very useful in order to study phase transitions in such problems [6]. The hardest among these share characteristics that are largely independent of the specific algorithms adopted for their solution. Important features such as solution time or memory requirements are conjectured to be strictly related to the geometrical structure of their low temperature phase space [7]. For a survey on the state of the art we address the reader to two recent special issues [8].

The main technical obstacle for the development of a statistical physics theory over finite degree graphs has been the extension of the Parisi replica symmetry breaking

(RSB) scheme to the functional level [9,10]. The replica symmetric (RS) phases are described by a single probability distribution function of the effective fields, capturing the site-to-site fluctuations of the local magnetization. On the contrary, when the symmetry among replicas breaks down, there appear many pure states, each one endowed with its own effective field distribution. The site-to-site fluctuations induce correlations among such probability distributions. The overall free energy has to be optimized in a large functional space which becomes more and more complex as the Parisi scheme is iterated. Recently in [11] a population dynamics algorithm has been introduced which is able, for large enough computer resources, to reconstruct the field distributions that lead to the numerical solution of the one-step RSB (1RSB) equations in full generality.

In this Letter we reexamine in the appropriate 1RSB context an ansatz previously introduced in [10] to get an approximated solution of the Viana-Bray model. That ansatz, which neglects site-to-site fluctuations, allows for great simplifications in the functional equations describing the low temperature regime of spin glasses and optimization problems defined on graphs with finite connectivity. The ansatz solves exactly the saddle-point equations for models defined over uniform degree random hypergraphs, and it is simple enough to allow for the explicit computation of the thermodynamic quantities at low temperature, which remarkably agree with numerics. As representative instances, we compute the ground state (GS) energy of the p -spin glass and of the Bicoloring problem. In both cases, the problem of finding the GS is a hard computational task (NP-hard). To the best of our knowledge, the one presented here is the first exact, fully analytical solution for diluted models in the RSB phase.

For the p -spin glass with fluctuating connectivities where site-to-site correlations are in principle important, the same ansatz allows one to evaluate exactly the configurational entropy and the dynamical and static transition points found as the average connectivity is increased

[12]. In computer science this model is known as random p -XOR-SAT [13] and its complete probabilistic characterization is considered an open problem (at present only lower and upper rigorous bounds to the critical threshold are known [14]). From a combinatorial standpoint this problem has straight connections with the well-studied domain of random linear systems over finite fields, with applications in coding and cryptography [15].

In the fluctuating connectivity framework, we have also tested the method as a variational approach to the study of the GS properties of random NP-complete combinatorial problems, such as random 3-SAT or Bicoloring [4], obtaining the currently most accurate analytical estimation of their critical SAT/UNSAT thresholds (see below).

In what follows we shall concentrate on the $p = 3$ spin interactions, the generalization to arbitrary p being straightforward. The Hamiltonian of the models we have chosen to study reads $H = \sum_{[i,j,k] \in E} G[S_i, S_j, S_k]$, where $S_i = \pm 1$ are Ising spins and E is the set of triples (plaquettes), which form a random hypergraph (locally the

graph has the topology of a Husimi tree). In the fixed connectivity case, every index $i = 1, \dots, N$ must appear in E the same number $k + 1$ of times. However, the presence of hyperloops [12] of length of the order $\log(N)$ induces nontrivial contributions to the free energy. In the fluctuating connectivity case, each possible plaquette is chosen at random with probability γ/N^2 .

In the three-spin glass case, the local interaction reads $G[S_i, S_j, S_k] = -J_{ijk} S_i S_j S_k$ with $J_{ijk} = \pm 1$ randomly. For the Bicoloring problem we have $G[S_i, S_j, S_k] = \delta(S_i, S_j) \delta(S_i, S_k) = \frac{1}{4}(S_i S_j + S_i S_k + S_j S_k + 1)$. Each interaction adds zero energy only if the spin configuration is not monochromatic; i.e., not all spins on the plaquette are equal. The optimization problem amounts to minimizing the number of monochromatic plaquettes.

First we focus on the fixed connectivity case (with connectivity $k + 1$). In order to calculate the averaged free energy at inverse temperature β we resort to the replica method, where the average free energy is evaluated from an analytic continuation of the integer moments of the partition function [1]. The replicated free energy reads

$$\beta f_n = \overline{Z}^n = \text{extr}_{f(\vec{\sigma})} \left[k \ln \left(\sum_{\vec{\sigma}} f(\vec{\sigma})^{\frac{k+1}{k}} \right) - \frac{k+1}{3} \ln \left(\sum_{\vec{\sigma}_1, \vec{\sigma}_2, \vec{\sigma}_3} f(\vec{\sigma}_1) f(\vec{\sigma}_2) f(\vec{\sigma}_3) e^{\beta \sum_{a=1}^n \mathcal{G}[\sigma_a^1, \sigma_a^2, \sigma_a^3]} \right) \right], \quad (1)$$

with $\mathcal{G}[x, y, z] = xyz$ for the spin glass and $\mathcal{G}[x, y, z] = -(xy + yz + xz + 1)/4$ for Bicoloring. $a = 1, \dots, n$ is the replica index, $\vec{\sigma} = \{\sigma^1, \dots, \sigma^n\}$ is a vector of n Ising variables, and $f(\vec{\sigma}) \propto c(\vec{\sigma})^k$, where $c(\vec{\sigma}) = N^{-1} \sum_i \delta(\tilde{S}_i - \vec{\sigma})$ counts the fraction of sites i having replicated spin $S_i^a = \sigma^a$. The functional order parameter $f(\vec{\sigma})$ must be symmetric in $\vec{\sigma}$. From Eq. (1) one obtains the following saddle point equations:

$$f(\vec{\sigma}) = \frac{D^k(\vec{\sigma})}{\sum_{\vec{\sigma}} D^k(\vec{\sigma})}, \quad (2)$$

$$D(\vec{\sigma}) = \sum_{\vec{\tau}, \vec{\mu}} f(\vec{\tau}) f(\vec{\mu}) \exp \left(\beta \sum_{a=1}^n \mathcal{G}[\sigma^a, \tau^a, \mu^a] \right). \quad (3)$$

The preceding equations admit a paramagnetic and a spin-glass solution. As long as replica symmetry holds (e.g., in the paramagnetic or ferromagnetic phases) the order parameter $f(\vec{\sigma})$ depends only on the sum $\sum_a \sigma^a$, i.e., on a single probability distribution of effective local fields. However, in the glassy phase the RS solution is not optimal (and yet stable), and one needs a RSB ansatz, which is in general very complicated, even in the simplest case of 1RSB. Nevertheless, in our case, the observation that the sites are locally equivalent suggests to neglect site-to-site fluctuations in the distribution of the effective fields. In the replica formalism this fact is reflected in the use of the following *factorized* ansatz [10,16]:

$$f(\vec{\sigma}) = \prod_{g=1}^{n/m} \tilde{f}(\vec{\sigma}_g) = \prod_{g=1}^{n/m} \int dh P(h) \frac{e^{\beta h \sum_{a=1}^m \sigma_g^a}}{(2 \cosh \beta h)^m}, \quad (4)$$

where the n replicas have been divided into n/m groups of m replicas each and $\vec{\sigma}_g$ is an m -dimensional vector with the components belonging to the g th group. The general

interpretation of the 1RSB order parameter [11] shows that $P(h)$ is the probability distribution of the cavity field, i.e., the field on a site after one of the interactions of that site has been removed. The above ansatz is consistent with the saddle-point equations (2) and (3), and the very same equations are verified by $\tilde{f}(\vec{\sigma}_g)$ and $\tilde{D}(\vec{\sigma}_g)$ with the sum in (3) running only up to m .

The RSB saddle-point equations are different for the two models. In the three-spin case we find

$$\frac{P(h)}{(2 \cosh \beta h)^m} = A_k^{-1} \int \prod_{i=1}^k \frac{du_i Q(u_i)}{(\cosh \beta u_i)^m} \delta \left(h - \sum_{i=1}^k u_i \right), \quad (5)$$

where $Q(u) = \int \mathcal{D}h \mathcal{D}g \delta[u - u(h, g)]$, with $\mathcal{D}h = dh P(h)$ and $\tanh[\beta u(h, g)] = \tanh(\beta) \tanh(\beta h) \tanh(\beta g)$, and A_k normalizes the $P(h)$. For Bicoloring we find

$$\frac{P(h)}{(2 \cosh \beta h)^m} = A_k^{-1} \int \prod_{i=1}^k \frac{\mathcal{D}h_i \mathcal{D}g_i W(h_i, g_i)^m}{[4 \cosh(\beta h_i) \cosh(\beta g_i)]^m} \times \delta \left(h - \sum_{i=1}^k t(h_i, g_i) \right), \quad (6)$$

where $t(h, g) = \frac{1}{2} \beta^{-1} \ln(\alpha_- / \alpha_+)$ and $W(h, g) = \sqrt{\alpha_- \alpha_+}$ with $\alpha_{\pm} = 2 \cosh[\beta(h - g)] + 2 \cosh[\beta(h + g \pm 1)] e^{-\beta}$. The RS (paramagnetic) equation is recovered for $m = n$ ($m = 1$). As usual, in order to find the thermodynamical free energy a maximization of the free-energy functional with respect to m should be performed.

For a generic temperature the solutions to (5) and (6) can easily be found numerically with a RS-like population dynamics, which requires much less computational effort than the 1RSB algorithm of Ref. [11].

Interestingly enough in the limit of zero temperature we can solve the equations analytically. Indeed, for $\beta \rightarrow \infty$ we have $u(h, g) \rightarrow \text{sgn}(hg) \min(1, h, g)$ and $t(h, g) \rightarrow -\text{sgn}(h) \min(1, h, g) \theta(hg)$ (where θ is the step function). Then both $u(h, g)$ and $t(h, g)$ can take only the values 0 and ± 1 for integer valued cavity fields. Rational valued solutions also exist and yet vanish close to the free-energy maximum.

For the p -spin with odd connectivity $k + 1$ and for the Bicoloring the analytical expressions are quite involved and will be given elsewhere [17]. For p spin with even connectivities (i.e., odd k) the solution can be written in a very compact way,

$$f_0(y, k + 1) = \frac{2k - 1}{3} g(y, k + 1) - \frac{2k + 2}{3} g(y, k), \quad (7)$$

$$\text{with } g(y, k) = \frac{1}{y} \ln \left[2^{-k} \sum_{i=0}^k \binom{k}{i} e^{y|k-2i|} \right],$$

where y is the zero temperature limit of the quantity βm which turns out to be finite. The GS energy (e_{gs}) corresponds to the maximum of f_0 [1]. For connectivities smaller than 4 for the p -spin and 7 for the Bicoloring, the maximum is always in $y = \infty$ and corresponds to the RS paramagnetic solution $P(h) = \delta(h)$. The RS spin-glass solution, located in $y = 0$, has always a lower energy with respect to the physical one. For some connectivities the free-energy values (e_{gs}) are reported in the tables, together with the corresponding $y = y^*$ saddle-point values. For the three-spin case we also report numerical estimations of the GS energy ($e_{\text{gs}}^{\text{num}}$) obtained by extrapolating the results of exhaustive enumerations (sizes up to $N = 60$ averaged over 1000–10000 samples). Moreover, in [18] the y^* value for the three-spin model with $k + 1 = 4$ has been estimated to be 1.41(1), perfectly compatible with our analytic value.

A further check of the analytic solution in the p -spin case is provided by the proper convergence, in the limit $k \rightarrow \infty$, to the exact solution of the fully connected p -spin model by Gardner [19] after a proper rescaling of the coupling.

Three-spin			
$k + 1$	e_{gs}	$e_{\text{gs}}^{\text{num}}$	y^*
1–3	$-(k + 1)/3$		∞
4	-1.217 71	-1.218(6)	1.411 55
5	-1.394 92	-1.395(7)	1.095 72
6	-1.544 14	-1.544(9)	0.901 63

Bicoloring		
$k + 1$	e_{gs}	y^*
1–6	0	∞
7	0.003 711	1.966 11
8	0.027 383	1.171 18
9	0.058 131	0.928 87
10	0.093 181	0.787 46
11	0.131 392	0.693 15
12	0.172 118	0.553 38

In the case of models defined over nonhomogeneous graphs the ansatz can be used to obtain approximate or, in some cases, exact variational estimates of the thermodynamic functions. We have considered three representative cases: the three-spin model and the Bicoloring problem over random hypergraphs with a Poisson distribution of site connectivities, and the random 3-SAT problem.

For the three-spin model we obtained estimates of the dynamical and static critical points looking at the *configurational entropy*. It has been shown in [12] that in this model the GS are clustered. Given a GS there is an exponential number of other GS which can be reached through GS paths where subsequent GS differ only by a finite number of spin flips. For small average connectivity there is a unique cluster, while above a threshold γ_d the number of disconnected clusters become exponentially large. The configurational entropy is the logarithm of the number of clusters per spin, and can be computed in the replica 1RSB formalism as $\Sigma(\gamma) = \frac{\partial f}{\partial m} |_{m=1}$ [20]. $\Sigma(\gamma)$ jumps to a nonzero value at the dynamical critical point γ_d , and then it vanishes again at the static critical point γ_s . Using arguments put forward in [21], one can show [17] that, due to the triviality of the paramagnetic phase of the model [12], where $P(h) = \delta(h)$, the factorized ansatz (4) yields the exact result. The resulting expression reads

$$\Sigma(\gamma) = \ln(2)[r - 3\gamma r^2(1 - r) - \gamma r^3], \quad (8)$$

with r solving the $m = 1$ saddle-point equation $1 - r = \exp(-3\gamma r^2)$. The above expression is different from zero between $\gamma_d = 0.818$ and $\gamma_s = 0.918$ (see bold line in Fig. 1) where it equals the difference between the paramagnetic and the ferromagnetic entropies [12]. The above critical points coincide with numerical estimates [12].

In this model the static RSB transition point γ_s coincides with the critical point γ_c beyond which the system becomes frustrated; that is, no longer can all interactions be satisfied at the same time, and therefore the GS

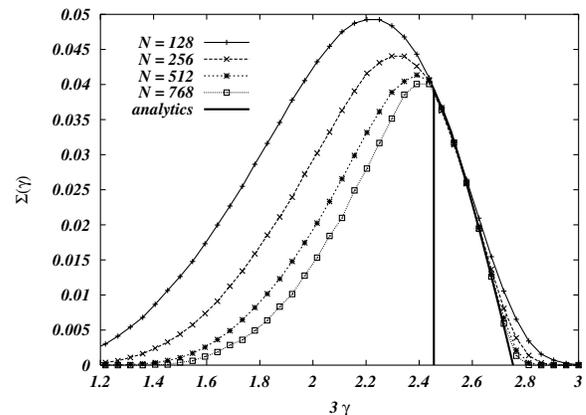


FIG. 1. Ground states configurational entropy versus mean connectivity for the three-spin model. The results of numerical clustering with an overlap cutoff of 0.7 (averaged over 1000, 1000, 500, and 50 samples) converge to the analytical prediction.

energy becomes positive [12]. In computer science this point is known as the SAT/UNSAT critical threshold: $\gamma_c = \gamma_s = 0.918$ thus provides the critical threshold for random 3-XOR-SAT, in perfect agreement with the numerical estimation [12].

Above γ_s the factorized ansatz ceases to be exact and can be used only at a variational level.

In order to check numerically Eq. (8), we have performed a GS clustering. This task is in general very hard due to the large number of GS and because of the lack of a proper definition of clusters in finite size systems. However, in this model calculations are easier, thanks to the presence of only two relevant overlaps between GS: The internal overlap equals r and is always larger than 0.7, while different clusters are almost orthogonal. This leads to an optimal cutoff of 0.7 for the numerical identification of clusters. The results shown in Fig. 1 are in remarkable agreement with the analytical curve.

Finally, in models where the configurational entropy is likely to be zero and correlation among clusters is stronger, like Bicoloring over fluctuating degree random graphs and 3-SAT [22], the dynamic and static critical points coincide ($\gamma_d = \gamma_s$) and precede the SAT/UNSAT critical point γ_c (usually called α_c). Though less effective, the factorized ansatz with integer valued fields still provides an estimate for γ_c [23]. Namely, $\gamma_c^{\text{var}} = 4.3962$ for 3-SAT and $\gamma_c^{\text{var}} = 2.149$ for Bicoloring, which improve present rigorous bounds (recently reviewed in [24]).

To summarize, we have studied a factorization ansatz which allows us to solve exactly diluted spin-glass and optimization models, on homogeneous hypergraphs. These analytical results can play a crucial role in testing convergence of heuristic algorithms. For nonhomogeneous graphs the ansatz still allows one to get very good results (some of them exact) as we have shown for the p -spin, the Bicoloring, and the 3-SAT problems. Encouraged by the recent rigorous results obtained on simpler models in [25,26], we trust that an alternative and mathematically rigorous derivation of our results may be possible.

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