

Rigorous Decimation-Based Construction of Ground Pure States for Spin-Glass Models on Random Lattices

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A constructive scheme for determining pure states at very low temperature in the 3-spins glass model on a random lattice is provided, in full agreement with Parisi's one step replica symmetry breaking (RSB) scheme. Proof is based on the analysis of a partial decimation procedure and of the statistical properties of its output, i.e., a reduced Hamiltonian acting on a subset of the initial spins. The number of ground states (GS) in each state, the number of states, and the distances between GS are calculated and correspond to RSB predictions.

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Parisi's replica symmetry breaking (RSB) theory and its physical interpretation have turned out to be very fruitful for the investigation of disordered systems over the past 20 years [1]. Unfortunately, the mathematical basis for RSB is rather weak. Rigorous studies confirming RSB predictions have been limited to few mean-field models thus far [2]. One of the most striking assumptions in RSB theory, the existence of numerous pure states, or clusters, in phase space on which the Gibbs measure becomes concentrated at low temperature is still not fully understood even at the mean-field level despite recent progress [2], not to mention its applicability to finite dimensional systems.

In this Letter, we present a rigorous study of a spin glass model which allows us to identify explicitly pure states for a given sample. Our analysis consists in decimating well chosen spins appearing in the original Hamiltonian H . When decimation stops, two cases may occur depending on the value of control parameters. If no spin is left, the partition function is entirely known, as well as the properties of H ; this situation corresponds to the existence of a single pure state and replica symmetry (RS). Otherwise, some reduced Hamiltonian H' involving a subset S' of the original set of spins S has to be treated. The ground states (GS) of H' can be interpreted as seeds for the (low temperature) pure states of H . More precisely, all GS in a pure state of H can be reconstructed when backtracking the original decimation procedure from the seed of this cluster. Analysis of the statistical properties of seeds in the S' space, and of the reconstruction process, provides a full characterization of the structure of GS in the S space.

The model we consider is the so-called 3-spins Ising spin glass. M triplets of distinct integers $i_m < j_m < k_m$ are randomly chosen in the range $1, \dots, N$; plaquette m , formed by the attached spins, is associated with a coupling J_m equal to ± 1 with equal probabilities. The

Hamiltonian

$$H = - \sum_{m=1}^M J_m S_{i_m} S_{j_m} S_{k_m} \quad (1)$$

equals $-M$ plus twice the number of frustrated plaquettes. We shall use c to denote the number of plaquettes per spin, M/N . The thermodynamical properties of model (1) were first investigated when all spins interact together, i.e., in the limit of large ratios c [3,4]. Three phases were found. When the temperature T is larger than $T_d(c) \sim 0.68\sqrt{c}$, the system is paramagnetic (RS phase) [4]. At low temperatures $T < T_s(c) \sim 0.65\sqrt{c}$ [3], the system is trapped in one of the few existing glassy pure states. In the intermediate range $T_s < T < T_d$, there exist an exponential number of glassy pure states, separated by infinite barriers [4].

As the ratio c of plaquettes (interactions) per spin decreases, so do the temperatures T_d and T_s . The ratios $c_d \simeq 0.818$ and $c_s \simeq 0.918$, at which they, respectively, vanish, have been calculated in the framework of one step RSB theory [5], with the following zero temperature picture [6]. For $c < c_s$ (respectively, $c > c_s$), the ground state (GS) of Hamiltonian (1) are unfrustrated (respectively, frustrated), i.e., have an energy per spin equal to (respectively, larger than) $-c$. In the unfrustrated phase, the number of GS scales as 2^{Ns} where the zero temperature entropy simply equals $s = 1 - c$ (base 2 logarithm) (Fig. 1). With high probability, two GS differ by a number of spins equal to Nd with $d = 1/2$. The spatial organization of GS in the space of configurations S (N -dimensional hypercube) undergoes a drastic change at c_d (Fig. 1), reminiscent of the ergodicity breaking taking place at $T_d(c)$. The set of GS breaks into a large number, 2^{Ns_0} , of clusters, each containing an exponential number, 2^{Ns_1} , of GS. Two GS belonging to different clusters lie apart at a typical Hamming distance $d_0 = d = 1/2$ while, inside

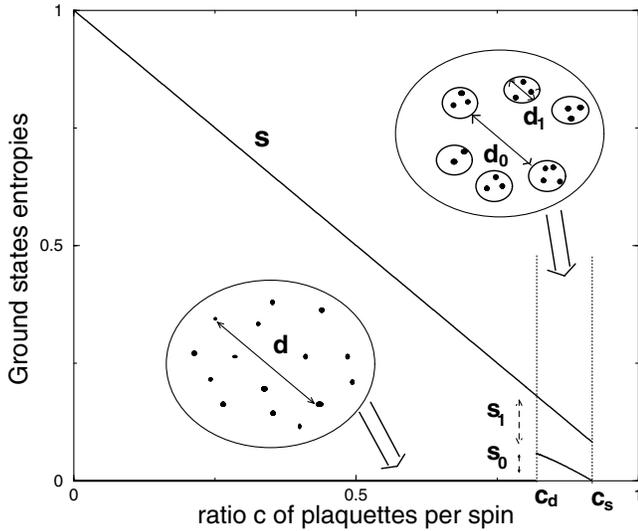


FIG. 1. GS structure and entropies as a function of the ratio c of plaquettes per spin. The total entropy (log number of unfrustrated GS per spin) is $s = 1 - c$ for $c < c_s \approx 0.918$. For $c < c_d \approx 0.818$, GS are uniformly scattered on the N -dimensional hypercube, with a typical normalized Hamming distance $d = 1/2$. At c_d , the GS space discontinuously breaks into disjoint clusters: The Hamming distance $d_1 \approx 0.14$ between solutions inside a cluster is much smaller than the typical distance $d_0 = 1/2$ between two clusters (RSB transition). The entropy of clusters, s_0 , and of solutions in each cluster, s_1 , are such that $s_0 + s_1 = s$. At c_s , the number of clusters ceases to be exponentially large ($s_0 = 0$). Above c_s , GS are frustrated.

a cluster, the distance is smaller, and equal to $d_1 = (1 - b)/2$. b , the largest root of

$$b = 1 - e^{-3cb^2}, \quad (2)$$

measures the size of the cluster backbone, i.e., the fraction of spins common to all GS in a cluster. The entropies of clusters, $s_0 = b - 3cb^2 + 2cb^3$, and GS in a cluster, $s_1 = s - s_0$, are shown in Fig. 1 [5]. At c_d , the total entropy s is analytic in c , while the order parameter b , the entropies s_0, s_1 undergo discontinuous (first order) jumps, e.g., from $b_d^- = 0$ to $b_d^+ \approx 0.71$.

We now sketch how the above results may be found back rigorously. The techniques used are borrowed from probability theory, and the analysis of algorithms. Their use was suggested from the close relationship between Hamiltonian (1) and the random 3-XORSAT optimization problem [5,7,8]. Let us call ℓ -spin a spin which appears in ℓ distinct plaquettes in (1). Plaquettes containing at least a 1-spin are never frustrated. Our decimation procedure consists in a recursive elimination of these plaquettes and attached 1-spins (Fig. 2), until no 1-spin is left [9]. We define the numbers $N_\ell(T)$ of ℓ -spins after T steps of the decimation algorithm, i.e., once T plaquettes have been removed, and their set $\mathcal{N}(T) = \{N_\ell(T), \ell \geq 0\}$.

The variations of the N_ℓ during the $(T + 1)$ th step of the algorithm are stochastic variables due to the randomness in (1) and the choice of the 1-spin to be removed, with conditional expectations with respect to $\mathcal{N}(T)$ given by

$$\begin{aligned} \mathbf{E}[N_\ell(T + 1) - N_\ell(T) | \mathcal{N}(T)] &= 2p_{\ell+1}(T) - 2p_\ell(T) \\ &+ \delta_{\ell,0} - \delta_{\ell,1}, \end{aligned} \quad (3)$$

where δ denotes the Kronecker function. When a plaquette is removed, a 1-spin disappears [$\delta_{\ell,1}$ term in (3)] to become a 0-spin ($\delta_{\ell,0}$). The plaquette contains two other spins. The number of occurrences ℓ of each of these two spins is distributed with probability $p_\ell(T) = \ell N_\ell(T)/3/(M - T)$, and is diminished by one once the plaquette is taken away. For large sizes N , the densities $n_\ell = N_\ell/N$ of ℓ -spins become self-averaging, and evolve on a long time scale of the order of N [10]. Defining the reduced time $t = T/N$, the densities obey a set of coupled differential equations which can be deduced from (3),

$$\frac{dn_\ell}{dt} = \frac{2[(\ell + 1)n_{\ell+1}(t) - \ell n_\ell(t)]}{3(c - t)} + \delta_{\ell,0} - \delta_{\ell,1}. \quad (4)$$

Initially, densities are Poisson distributed: $n_\ell(0) = e^{-3c} (3c)^\ell / \ell!$. Equation (4) may be solved, with the result

$$n_1(t) = 3cb(t)^2 [e^{-3cb(t)^2} + b(t) - 1], \quad (5)$$

where $b(t) \equiv (1 - t/c)^{1/3}$, while $n_\ell(t)$ is given by a Poisson distribution of parameter $3cb(t)^2$ for $\ell \geq 2$. The density of 1-spins is shown in Fig. 3 for various initial plaquettes per spin ratios c . The algorithm stops at the time t^* for which n_1 vanishes, that is, when no 1-spin is left. From Eq. (5), $b(t^*)$ coincides with b defined in Eq. (2) [11].

What does the reduced Hamiltonian H' look like once the decimation has stopped? For $c < c_d$, $t^* = c$, and no spin and plaquette is left. The entropy s of GS of H can be

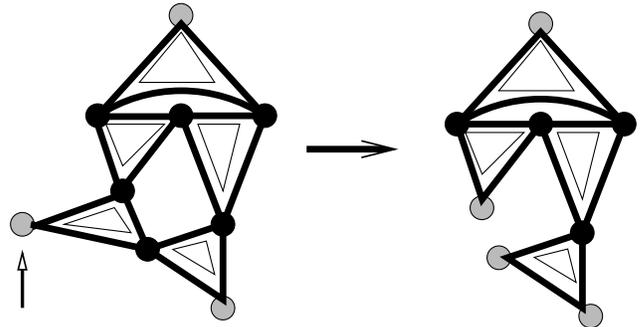


FIG. 2. Graph representation of the 3-spins Hamiltonian. Vertices (spins) are joined by plaquettes (values ± 1 of couplings are not shown here). A step of decimation consists in listing all 1-spins (gray vertices), choosing randomly one of them (gray vertex pointed by the arrow), and eliminating this spin and its plaquette. New 1-spins may appear. Decimation is repeated until no 1-spin is left.

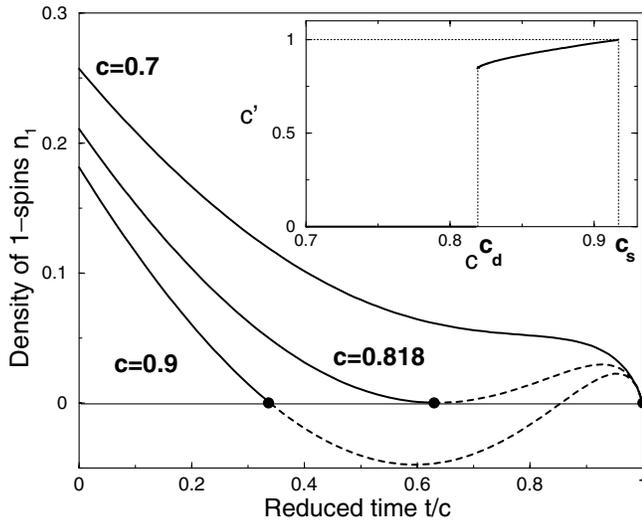


FIG. 3. Evolution of the density of 1-spins $n_1(t)$ generated by the decimation procedure. For $c < c_d \approx 0.818$, $n_1(t)$ remains positive until all the plaquettes are eliminated at $t^* = c$. For $c > c_d$, the decimation procedure stops at the time t^* for which n_1 vanishes (black dots), and the solution of Eq. (4) is non-physical for $t > t^*$ (dashed part of the curves). Notice that t^* discontinuously jumps down at $c = c_d$ (first order transition). Inset: Plaquette density c' for the reduced Hamiltonian H' vs c . At $c = c_d$, c' discontinuously jumps to a positive value; the threshold $c' = 1$ for the disappearance of unfrustrated GS is reached for $c_s \approx 0.918$.

computed recursively. Each time a plaquette containing $\nu (\geq 1)$ 1-spins and these ν vertices are removed (Fig. 2), the number of GS gets divided by $2^{\nu-1}$, and the average entropy (base 2 logarithm) of GS decreased by $\mathbf{E}[\nu - 1 | \mathcal{N}(T)] = 2 p_1(T)$. As no spin is left when the algorithm stops, the final value for the entropy vanishes, giving

$$s = \int_0^{t^*} dt \frac{2n_1(t)}{3(c-t)} + e^{-3c}, \quad (6)$$

where the last term comes from the contribution $n_0(0)$ of 0-spins. Using Eq. (5) and $t^* = c$, we find back $s = 1 - c$. When $c_d < c < c_s$, the decimation procedure stops at $t^* < c$, and has not succeeded in eliminating all plaquettes and spins. The remaining fraction of plaquettes per spin, $c' = (c - t^*)/\sigma$, where $\sigma = \sum_{\ell \geq 2} n_\ell(t^*)$, is plotted as a function of c in the inset of Fig. 3. Each GS of H' can be seen as a seed from which a cluster of GS of H in the original configuration space can be reconstructed. To do so, plaquettes which were eliminated during decimation are reintroduced, one after the other, and the spins they contain are assigned all possible values that leave the plaquettes unfrustrated. Combining any of these partial spin assignments with (free) 0-spin assignments, all the GS in a cluster are obtained. Repeating the argument leading to the calculation of the entropy in the $c < c_d$

case, we find that the average entropy s_1 of GS in a cluster is given by the right-hand side of Eq. (6), and agrees with the RSB prediction.

To complete the description of clusters, some statistical knowledge about their seeds is required. The number \mathcal{U}' of GS of H' can be analyzed by means of the first and second moments method [12], giving, respectively, some upper and lower bound to the probability $\Pr(\mathcal{U}' \geq 1)$ of existence of unfrustrated GS,

$$\frac{\mathbf{E}(\mathcal{U}')^2}{\mathbf{E}(\mathcal{U}'^2)} \leq \Pr(\mathcal{U}' \geq 1) \leq \mathbf{E}(\mathcal{U}'). \quad (7)$$

The right inequality is a consequence of the Markov bound for positive variables, $\Pr(\mathcal{U}' \geq a) \leq \mathbf{E}(\mathcal{U}')/a$, with $a = 1$, while the left inequality can be established from the Cauchy-Schwarz inequality, $\mathbf{E}(\mathcal{U}' \cdot \mathcal{V})^2 \leq \mathbf{E}(\mathcal{U}'^2) \cdot \mathbf{E}(\mathcal{V}^2)$, taking $\mathcal{V} \equiv 1 - \delta_{\mathcal{U}',0}$. As shown below, the lower and upper bounds to the threshold c'_s separating unfrustrated and frustrated phases obtained from Eq. (7) coincide, which allows an exact determination of c'_s .

In the limit of a large number N' of nondecimated spins, the first moment depends only on the numbers of spins and plaquettes: $\mathbf{E}(\mathcal{U}') = 2^{N'(1-c')}$. From (7), we conclude that \mathcal{U}' almost surely vanishes when $c' > 1$. On the contrary, the second moment is affected by the existence of constraints on the minimal number (two) of occurrences of spins in H' . Its computation requires a combinatorial analysis of the number of Hamiltonians H , i.e., ways of choosing plaquettes and couplings in (1), having a given pair of configurations for GS. As this number depends only on the distance d' between the two configurations, $\mathbf{E}(\mathcal{U}'^2)$ may be expressed as a combinatorial sum involving level-2 generalized Stirling numbers of the second kind, i.e., the number of ways to partition objects (spins in plaquettes) into subsets (spin indices) having each at least two elements [8]. Very general asymptotic estimates for these have recently been found, which involve parameters implicitly defined by transcendental saddle-point equations [13]. In the present case and for $c' < 1$, our sum has just one dominant exponential term, which is precisely the square of the first moment, $4^{N'(1-c')}$. This statement remains true when nonexponential (in N) contributions to the moments are calculated. So, for $c' < 1$ and $N' \rightarrow \infty$, the left-hand side of (7) is asymptotically equal to unity, and GS are almost surely unfrustrated. The value c_s of c giving $c' = 1$ is found from the analysis of the algorithm (inset of Fig. 3) to be ≈ 0.918 . In addition, the entropy $s'_0 = 1 - c'$ of GS allows one to find back the RSB expression for the entropy of clusters, $s_0 = \sigma s'_0$.

The self-averageness of \mathcal{U}' , i.e., of the partition function $Z' \approx \mathcal{U}' e^{M'/T}$ in the low temperature $T \rightarrow 0$ limit, contrasts with the (sample-to-sample) fluctuations exhibited by \mathcal{U} . Indeed, a direct application of inequalities

(7) to \mathcal{U} only permits to derive upper ($c_s \leq 1$) and lower ($c_s \geq 0.889$) bounds to the threshold [7]. Fluctuations of \mathcal{U} thus essentially come from fluctuations in the numbers of 0- and 1-spins (whose plaquettes form the dangling ends of the graph in Fig. 2) removed by the decimation algorithm. Conversely, in H' , spins appear at least twice and are more interconnected, giving rise to weaker fluctuations for \mathcal{U}' .

The reconstruction process allows a complete characterization of GS, in terms of an extensive number of (possibly overlapping) blocks made of few spins, each block being allowed to flip as a whole from a GS to another. When $c < c_d$, with high probability, two randomly picked GS differ over a fraction $d = 1/2$ of spins, but are connected through a sequence of $O(N)$ successive GS differing over $O(1)$ spins only. For $c_d < c < c_s$, flip-pable blocks are juxtaposed to a set of seed-dependent frozen spins. To prove the existence of clustering predicted by RSB (Fig. 1), we have checked that the largest Hamming distance d_1^{\max} between two GS associated to the same seed is lower than the smallest possible distance d_0^{\min} between GS reconstructed from two different seeds. We have estimated d_0^{\min} as a function of c using again the first moment method, i.e., from the vanishing condition of the expectation number $\mathbf{E}(\mathcal{U}^2|d_0)$ of GS lying apart at distance $\leq d_0$. As for d_1^{\max} , each time a plaquette with $v \geq 2$ 1-spins is reintroduced, the distance between reconstructed GS increases by $2/N$ at most, leading to $d_1^{\max} \leq 2 \int_0^{t^*} dt p_1(2 - p_1) + e^{-3c}$.

The above results may be extended to multi- p -spin interactions with $p \neq 3$, with results in agreement with replica theory: The $p \geq 4$ case is qualitatively similar to $p = 3$; for $p = 2$, $c_d = c_s = 1/2$ both coincide with the percolation threshold. Another extension regards finite temperature. For $c < c_d$, the decimation algorithm allows a complete calculation of the free energy. Whether 1-spins are set to frustrate, or unfrustrate, the plaquette they belong to, the energy is increased, or decreased by one. The resulting free energy density equals $f(T) = -T \ln 2 - cT \ln \cosh(1/T)$ in agreement with the replica paramagnetic calculation [5]. The same expression for f is likely to be established for $c_d < c < c_s$ through an extension of the above approach. Investigation of the frustrated region, $c > c_s$, is currently under way, and would ultimately permit a rigorous construction of the continuous RSB phase. Our results also shed some light on the observed coincidence between the onset of RSB and the failure of a leaf removal algorithm in the vertex covering of random graphs [14]. Finally, it would be interesting to see how our spin decimation approach could be extended to other distributions of random lattices.

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