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From inherent structures to pure states: Some simple remarks and examples

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Abstract. – The notions of pure states and inherent structures, *i.e.* stable configurations against 1-spin flip are discussed. We explain why these different concepts accidentally coincide in mean-field models with infinite connectivity and present an exactly solvable one-dimensional model where they do not. At zero temperature pure states are to some extent related to k-spin flip stable configurations with $k \to \infty$ after the thermodynamical limit has been taken. This relationship is supported by an explicit analysis of the TAP equations and calculation of the number of pure states and k-spin flips stable configurations in a mean-field model with finite couplings. Finally, we discuss the relevance of the concepts of pure states and inherent structures in finite-dimensional glassy systems.

Introduction. – In a series of seminal papers, Kirkpatrick, Thirumalai and Wolynes (KTW) suggested ten years ago that (discontinuous) mean-field spin glasses could serve as a paradigm for vitreous systems [1]. The major success of KTW theory lies in its ability to predict the existence of both low (Kauzmann) and high (dynamical freezing) temperature critical points and thus to describe in a unified framework the thermodynamical and dynamical signatures of the glassy transition [2]. This achievement relies on a simple but rich picture of glassy *pure states* (PS), that is local minima in the *free-energy* landscape, and of the dynamical evolution taking place in the latter. To what extent KTW mean-field picture applies to real systems is a crucial issue [3, 4].

An apparently related approach based on the investigation of the *potential energy* landscape and of its local minima called *inherent structures* (IS) had been already proposed at the beginning of the eighties by Stillinger and Weber in the context of liquid theory [5]. IS present a considerable advantage with respect to PS: they are well defined and free of any mean-field hallmark. Recently, numerical studies proposing that some understanding of the glass transition could be gained from the analysis of potential energy landscapes [6] strengthened the feeling that Stillinger and Weber's analysis and KTW theory were basically the same description of glassy systems. This point of view was later supported by the equivalence of IS and PS in some mean-field spin-glasses, *e.g.*, Sherrington-Kirkpatrick (SK) or p-spins models [7] and by analytical works [3, 8].

In this letter, we present some arguments to clarify the relationship between IS and PS. We present some one-dimensional models for which IS can be exactly computed and do not

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coincide with PS. We show in addition that the degeneracy between IS and PS in infinitely connected models is due to the vanishing of the interactions in the thermodynamical limit and is lifted by the introduction of finite couplings. Focusing on the TAP equations "defining" PS and the number of the latter, we show that zero-temperature PS are related to extended IS, that is configurations stable with respect to an arbitrary large number k of spin flips (and not only to a single one as usual IS) [9].

Definitions and notations. – We consider a model including N Ising spins S_i. A configuration of spins will be said k-stable if its energy cannot be decreased by flipping any subset of k (or less than k) spins. Let us call $s_k(e)$ the logarithm (divided by N) of the number of k-stable configurations with energy density excess $e - e_{\rm GS}$ with respect to the ground state energy density $e_{\rm GS}$ when $N \to \infty$. IS correspond to 1-stable configurations and $s_1(e)$ is usually called configurational entropy. We have, of course, $s_{k+1}(e) \leq s_k(e)$ and $s_k(e) = -\infty$ for $e < e_{\rm GS}$.

The notion of PS is much trickier. In mean-field systems PS are usually defined through TAP equations [10] for the local magnetisations m_i. TAP solutions are exponentially numerous in the volume N and can be accounted for through the so-called complexity $\sigma(f)$, that is the normalised logarithm of PS having free-energy densities f. We shall focus in the following on the zero-temperature limit of the complexity $\sigma(e)$ and compare it to $s_k(e)$.

We shall denote hereafter the maximum over e of $s_k(e)$ (respectively, $\sigma(e)$) by s_k (respectively, σ).

One-dimensional disordered chain. – We first consider an Ising chain with disordered nearest-neighbour couplings L_i and no external field [11]. The L_i's are independent random variables drawn from an even distribution $P(L)$. No phase transition can take place at finite temperature: there is only one paramagnetic PS [11]. Therefore, the zero-temperature limit of the complexity simply reads $\sigma(e) = 0$ if $e = e_{\rm GS}$, $\sigma(e) = -\infty$ if $e \neq e_{\rm GS}$, where the ground state energy density equals $e_{\rm GS} = -\int {\rm d}L P(L)|L|$.

Ettelaie and Moore have calculated $s_1(e)$ [12]. We extend their approach to obtain $s_k(e)$ using the following observation by Li: a necessary and sufficient condition for a configuration to be k-stable is that each frustrated bond be k-weak, *i.e.* smaller in magnitude than the $2k$ nearest bonds (k on the left, k on the right) on the chain [13]. The typical and self-averaging $s_k(e)$ thus reads

$$s_k(e) = \lim_{N\to\infty} \frac{1}{N} \ln \left(\sum_{\{\tau_\ell = 0,1\}} \delta \left(e - e_{\rm GS} - \frac{2}{N} \sum_{\ell=1}^{N_k} |L_\ell| \tau_\ell \right) \right), \tag{1}$$

where N_k is the number of k-weak bonds on the chain and τ_ℓ equals 1 if the ℓ^{th} k-weak bond is frustrated, 0 otherwise. Using an integral representation of the delta function in (1), the τ_ℓ's may be traced over and one finds

$$\begin{aligned} s_k(e) \;&=\; \lim_{N\to\infty} \frac{1}{N} \ln \left\{ \int_{-i\infty}^{+i\infty} \frac{{\rm d}u}{2\pi N i} \times \right. \\ &\left. \times \;\exp\left[N \left(u(e - e_{\rm GS}) - 2 \int_0^{+\infty} {\rm d}L \; P_k(L) \; \ln(1 + e^{2Lu}) \right) \right] \right\}, \end{aligned} \tag{2}$$

where $P_k(L) = P(L)(2\int_{|L|}^{\infty} {\rm d}L' \; P(L') \;)^{2k}$ denotes the probability that a bond is k-weak and has value L. The integral over u can be evaluated by the method of steepest descent. In fig. 1, $s_k(e)$ is plotted for a Gaussian $P(L)$ (with variance unity) and for different values of

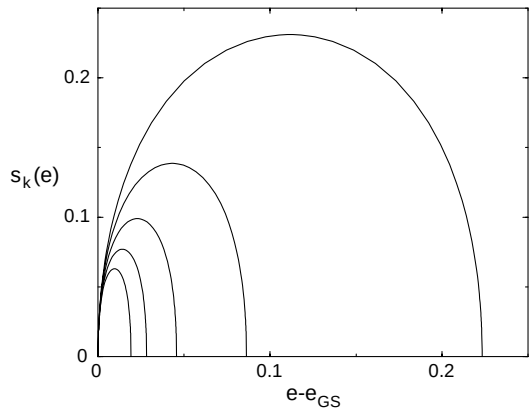

Fig. 1 – Logarithm of the number of k-stable configurations $s_k(e)$ as a function of the excess of energy density $e - e_{\rm GS}$ for a Gaussian coupling distribution $P(L)$ (with variance unity and zero mean). From top to bottom: $k = 1, 2, 3, 4, 5$.

k. At fixed k, $s_k(e)$ is symmetric around its maximum located in $e_k = e_{\rm GS} + \int {\rm d}L P_k(L)|L|$, $s_k = \ln 2/(2k+1)$. Note that the height of the maximum s_k, related to the total number of k-stable configurations is independent of P as found by Li [13]. On the left boundary, all curves exhibit an infinite slope when $e \to e_{\rm GS}$. More precisely, $s_k(e_{\rm GS} + \varepsilon) \propto -\varepsilon \ln \varepsilon$ if the support of $P(L)$ does not contain $L = 0$ and $s_k(e_{\rm GS} + \varepsilon) \propto \varepsilon^{(\alpha+1)/(\alpha+2)}$ if $P(L) \propto L^\alpha$ when $L \to 0$ (with $\alpha > -2$ to make $e_{\rm GS}$ finite).

The above model is a clear example of a system with many IS and at the same time a single PS. More precisely, the zero-temperature limit of the complexity $\sigma(e)$ (related to PS) is not equal to the configurational entropy $s_1(e)$ counting IS but to $s_\infty(e)$. Before exposing why s_1 and σ accidentally coincide in infinitely connected spin-glasses, let us briefly see to what extent the above results apply to generic finite-dimensional systems.

General remarks for finite-dimensional systems. – The main features of $s_k(e)$ can be found by some general arguments which apply to any *finite-dimensional* system. The behaviour of $s_1(e_{\rm GS} + \varepsilon)$ at small ε has been predicted in [14,15] and depends only on the lowest-lying excitations of the system. In addition, the scaling of the right-edge energy $2e_k - e_{\rm GS}$ at which $s_k(e)$ vanishes can be understood by a simple energy balance argument. Flipping a cluster of k spins among a configuration with energy density e, one may gain a bulk energy $E_{\rm b}(k) \sim -k(e - e_{\rm GS})$ and lose at least some surface energy $E_{\rm s}(k)$. As a consequence, k-stable configurations with energy densities higher than $e_{\rm GS} + E_{\rm s}(k)/k$ should not exist. For 1D Ising disordered chain, $E_{\rm s}(k)$ is equal to the average magnitude of the smallest bond among k ones and can be easily computed. As expected, $E_{\rm s}(k)/k \sim e_k - e_{\rm GS}$ for large k. Let us emphasise that the previous argument implies that there cannot be ∞-stable configurations (after the thermodynamical limit has been taken) with energy densities differing from the ground state one: $s_\infty(e \neq e_{\rm GS}) = -\infty$.

Mean-field spin-glasses with infinite connectivity. – It is well known that the zero-temperature limit of the complexity equals the configurational entropy in infinite connectivity spin-glasses [16]. For instance, in the case of the SK model,

$$\sigma^{\rm SK} = s_1^{\rm SK} = \max_z \left\{ -\frac{z^2}{2} + \ln 2 \int_{-z}^{+\infty} Dy \right\} \simeq 0.1992, \tag{3}$$

with $Dy \equiv e^{-y^2/2}/\sqrt{2\pi}\ \mathrm{d}y$ [17,18]. The equivalence between TAP solutions at zero temperature and 1-stable configurations (IS) is a straightforward consequence of the vanishing of couplings in the thermodynamical limit. The scaling of the couplings J_{ij} with size N ensures that the excitation energy ΔE_i, corresponding to flipping spin i remains finite in the thermodynamical limit, *e.g.*, $J_{ij} = \mathrm{O}(1/\sqrt{N})$ for the SK model. As a consequence, the excitation energy $\Delta E_{ij} = \Delta E_i + \Delta E_j - 2J_{ij}S_iS_j$ corresponding to flipping both spins i and j reduces to $\Delta E_i + \Delta E_j$ in the large-N limit. For infinite connectivity models IS are also k-stable configurations for every finite k. Therefore, $s_k(e)$ does not depend on k and $s_1 = \ldots = s_\infty = \sigma$.

TAP solutions at zero temperature are ∞-stable configurations. – We now show that in the presence of finite couplings, the degeneracy between all s_k's is lifted since k-stable configurations are not necessarily $k+1$-stable. In addition, we show that zero-temperature TAP solution are ∞-stable and not only 1-stable. To do so, let us first recall how TAP equations can be derived for a one-dimensional spin glass [19]. We call l_i and r_i, respectively, the effective magnetic fields due to all the spins on the left and on the right of i and h_i the external magnetic field acting on S_i. It is easy to write the equation verified by m_i in terms of l_{i-1} and r_{i-1},

$$m_i = \tanh\left[\beta h_i + \tanh^{-1}(\tanh(\beta l_{i-1})\tanh(\beta J_{i-1})) + \tanh^{-1}(\tanh(\beta r_{i+1})\tanh(\beta J_i))\right]. \quad (4)$$

This is the equation verified by the local magnetisation of a spin S_i interacting with two spins S_{i-1}, S_{i+1} on which the magnetic fields l_{i-1} and r_{i+1} act. Focusing on two neighbouring spins the equations verified by the two local magnetisations are

$$m_i = \frac{\tanh(\beta l_i) + \tanh(\beta J_i)\tanh(\beta r_{i+1})}{1 + \tanh(\beta l_i)\tanh(\beta J_i)\tanh(\beta r_{i+1})}, \quad (5)$$

$$m_{i+1} = \frac{\tanh(\beta r_{i+1}) + \tanh(\beta J_i)\tanh(\beta l_i)}{1 + \tanh(\beta l_i)\tanh(\beta J_i)\tanh(\beta r_{i+1})}. \quad (6)$$

These equations give m_i and m_{i+1} as a function of l_i and r_{i+1}. Inverting (5), (6) one obtains l_i and r_{i+1} as functions of m_i and m_{i+1}. Plugging $l_{i-1} = l_{i-1}(m_{i-1}, m_i)$ and $r_{i+1} = r_{i+1}(m_i, m_{i+1})$ into (4) the TAP equations for the local magnetisations are established [19].

To prove that TAP solutions are mapped into ground states in the zero-temperature limit, let us focus on k contiguous spins on the chain. The TAP equations on these k spins are by construction the equations verified by the local magnetisations of the system of k spins, as if it were isolated from the rest of the chain and there were magnetic fields l_{i_-}, r_{i_+} acting on the leftmost and rightmost spins, respectively. As a consequence, in the zero-temperature limit, the k local magnetisations tend towards the configuration of k spins which realizes the global minimum of the isolated system of k spins for any value of l_{i_-} and r_{i_+}. As k can be made arbitrarily large once N has been sent to infinity, the configurations corresponding to the zero-temperature limit of TAP solutions are ∞-stable. The argument can be straightforwardly extended to Ising spin glasses on Cayley trees or on random graphs.

Calculation for a mean-field model with finite couplings. – The results of the previous sections suggest that in finite connectivity models s_k is a non-trivial function of k which tends towards the zero-temperature limit of the complexity σ for large values of k. To corroborate this point, it is interesting to study a model whose complexity σ is non-zero. Consider the Hamiltonian $H = -\sum_{i<j} J_{ij}S_iS_j - \sum_{i=1}^{N} L_iS_iS_{i+1}$. The first term is the usual SK Hamiltonian: couplings J_{ij} are independent Gaussian random variables of zero mean and variance J^2/N. The one-dimensional Hamiltonian involves disordered interactions L_i which are independent random variables vanishing with probability $1-\alpha$ and distributed according to an

even distribution law $P(L)$ with probability α. This system smoothly interpolates between the SK model ($\alpha = 0$) and the one-dimensional spin glass ($J = 0$). We calculate below the departures of σ and s_k from their common value in the SK model to the first order in α only to avoid useless tedious calculations.

To compute the complexity two approaches can be used. The first one consists in making the (annealed) sum over all locally stable TAP solutions [17]. The other method relies on the computation of the logarithm of the (average) n-th power of the partition function using Bray and Moore replica symmetry breaking scheme [20]. As n goes to zero, the annealed complexity is recovered [21]. Calculations are sketched in appendices A and B and provide the same average complexity $\sigma(\alpha) = \sigma^{\rm SK} + \alpha\,\gamma^{(1)} + {\rm O}(\alpha^2)$, where

$$\gamma^{(1)} = -1 + \left(\int_{-\infty}^{+\infty} {\rm d}LP(L) \int_{-z^*-L/J}^{+\infty} Dy_1 Dy_2\; \theta(y_1 + y_2 + 2z^*) \right) \Big/ \left(\int_{-z^*}^{+\infty} Dy \right)^2 \qquad (7)$$

and $z^* \simeq 0.506$ is the maximum of (3). θ denotes the Heaviside function.

We now turn to the computation of s_k. The excitation energy corresponding to k-spin flips depends on the SK couplings and the initial configuration through the variables $x_i = \sum_{j(\neq i)} J_{ij} S_i S_j$ only. For large N, the x_i's become independent of the spin configuration $\{S_i\}$ and can be written as $x_i = y_i + z$, where y_i and z are independent Gaussian random variables of zero means and variances J^2 and J^2/N, respectively [22]. The annealed configurational entropy is defined through

$$e^{N s_1} = \left\langle \sum_{\{S_i\}} \prod_{i=1}^{N} \theta\left(L_{i-1} S_{i-1} S_i + L_i S_i S_{i+1} + y_i + z\right) \right\rangle_{\{L,y,z\}} . \qquad (8)$$

Once the average $\langle\cdot\rangle$ over disorder has been carried out, spins may be traced over and (8) may be evaluated for large N by the method of steepest descent. We find $s_1(\alpha) = \sigma^{\rm SK} + \alpha\, c_1^{(1)} + {\rm O}(\alpha^2)$ with

$$c_1^{(1)} = -1 + \left(\int_{-\infty}^{+\infty} {\rm d}LP(L) \int_{-z^*-L/J}^{+\infty} Dy_1 Dy_2 \right) \Big/ \left(\int_{-z^*}^{+\infty} Dy \right)^2 , \qquad (9)$$

giving $s_1 > \sigma$ as expected, compare (7) and (9) [23]. Repeating the same calculation for $k(\geq 2)$-stable configurations, we have found that they are equally numerous to the first order in α: $s_k(\alpha) = \sigma^{\rm SK} + \alpha\, c_k^{(1)} + {\rm O}(\alpha^2)$, with $c_k^{(1)} = \gamma^{(1)}$ for any $k \geq 2$. This result extends to higher orders in α as follows. Let us call $c_k^{(n)}$ the coefficient of α^n in s_k. Contributions to $c_k^{(n)}$ come from disordered lattices of L bonds involving clusters of at most $n+1$ contiguous spins along the chain. Clearly, spin configurations on such lattices that are $n+1$-stable are for ever stable. Therefore, $c_1^{(n)} > c_2^{(n)} > \ldots > c_{n+1}^{(n)} = c_k^{(n)}$ for any $k \geq n+1$. We have in particular explicitely checked that $c_2^{(2)} > c_3^{(2)}$.

As a conclusion, we have found a mean-field model with non-zero complexity σ and $s_1 > \sigma$. We have checked that σ coincides with s_∞ to the first order in the density of O(1) couplings.

Conclusion. – The above examples have shown the differences between IS and PS even in mean-field models provided that finite couplings are present. Our results could also be extended to models with continuous degrees of freedom, *e.g.* systems of N interacting particles [15]. In this case IS are configurations stable against *infinitesimal* moves of any subset of the N particles, that is local minima of the potential energy. k-stable local minima can be defined as IS stable against *finite* moves of any subset of k (or less than k) particles. ∞-stable minima gather all configurations that can be reached from each other by crossing finite barriers and are related to PS.

From the equilibrium point of view, PS and thus complexity are the only relevant concepts. The decomposition of the partition function put forward by Stillinger based on IS though mathematically exact does not seem to be thermodynamically founded [14]. However, usual nucleation arguments imply that no PS with free energy $f \neq f_{\rm eq}$ can live forever, that is $\sigma(f \neq f_{\rm eq}) = -\infty$. We thus face the following alternative. Either nucleation arguments break down for some reason and finite-dimensional glassy systems with full curves for $\sigma(f)$ may exist [3,8]. Or they hold and the KTW entropy crisis scenario cannot be extended to realistic systems without taking into account the notion of lifetime for PS (as was already emphasized in [1]). IS, besides their phenomenological interest, can be seen as a very valuable step in that direction.

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Appendix A. – To first order in α spin i has at most one neighbour $v = i \pm 1$ along the chain of L bonds. As a consequence, the TAP equations can be written as

$$m_i = \frac{t_i + t_v \tanh(\beta L)}{1 + t_i t_v \tanh(\beta L)} \ , \quad \tanh^{-1}(t_i) = \beta \sum_{j(\neq i)} J_{ij} m_j - \beta^2 J^2 (1-q) m_i \quad , \tag{10}$$

where $q = 1/N \sum_{i=1}^{N} m_i^2$. To compute the annealed complexity, we sum over all solutions of eqs. (10) following [17]. Introducing auxiliary variables, one can perform the average over J_{ij} and using the same notation as [17], we find

$$\begin{aligned} \sigma \ &= \ \mathrm{extr}_{q,\lambda,\Delta} \Bigg\{ - \lambda q - \Delta(1-q) - \Delta^2/2\beta^2 J^2 + \\ &+ \ \frac{1}{N} \ln \left\langle \int_{-1}^{+1} \prod_{i=1}^{N} \frac{\mathrm{d}t_i}{\beta J \sqrt{2\pi q}} \frac{1}{1-t_i^2} \exp\left[- \frac{(\tanh^{-1} t_i - \Delta m_i)^2}{2\beta^2 J^2 q} + \lambda m_i^2 \right] \right\rangle_{\{L\}} \Bigg\}. \end{aligned} \tag{11}$$

Performing the average on L_i at the first order in α and taking the zero-temperature limit, we obtain the expression of γ.

Appendix B. – To compute the n-th moment of the partition function, we use the replica trick and obtain n coupled chains. Defining the overlap q^{ab} between replicas a and b and the $2^n \times 2^n$ transfer matrix,

$$\begin{aligned} \mathcal{M}(\vec{S}, \vec{T}) \ &= \ \left\{ 1 - \alpha + \alpha \int \mathrm{d}L P(L) \exp\left[\beta L \sum_a S^a T^a \right] \right\} \times \\ &\times \ \exp\left[\frac{\beta^2 J^2}{2} \sum_{a<b} q^{ab} (S^a S^b + T^a T^b) \right] \ , \end{aligned} \tag{12}$$

the complexity may be computed within Bray and Moore two-group Ansatz [20]: $\sigma = \mathrm{extr}_{\{q\}}[-(\beta J)^2 \sum_{a<b} (q^{ab})^2/2 + \ln \Lambda(\{q\})]$, where $\Lambda(\{q\})$ is the largest eigenvalue of $\mathcal{M}$. The saddle-point equation for $\{q\}$ reads $q^{ab} = \sum_{\vec{S}} S^a S^b [\Psi(\vec{S})]^2$. The normalised ground state wave function Ψ obeys the two group symmetry with breakpoint m [20]. Ψ depends on $\vec{S} = (S^1, \ldots, S^n)$ through $S_- = \sum_{a \leq m} S^a$ and $S_+ = \sum_{a>m} S^a$ only and can be written as $\Psi(S_-, S_+) = c \int \mathrm{d}h_0 \mathrm{d}h_1 \rho(h_0, h_1) \exp[\beta h_0 (S_+ + S_-) + h_1 (S_+ - S_-)]$, where c is a normalisation factor. In the zero-temperature limit, the effective fields h_0, h_1 are both of order one and the

overlaps q^{ab} read $q_1 = A - z/(\beta mJ), q_2 = A - w/(\beta mJ)^2, q_3 = A + z/(\beta mJ), A \to 1$ with the notations of [20]. The eigenvalue equation for Λ, Ψ provides a linear equation for the effective field distribution

$$\lambda\rho(h_0,h_1) = \int \mathrm{d}LP(L)\Big\{(1-\alpha)\delta(L)+\alpha P(L)\Big\}\int DuDv\int \mathrm{d}h_0'\mathrm{d}h_1'\exp\left[h_1'\omega_L(h_0')\right]\times$$
$$\times\ \rho\Big(h_0'-Ju,h_1'-uz-v\sqrt{2w-z^2}\Big)\,\delta\Big(h_0-\varphi_L(h_0')\Big)\,\delta\Big(h_1-h_1'\eta_L(h_0')\Big), \quad (13)$$

where $\lambda = \Lambda\exp[\beta Jmz]$. $\omega_L(x)$ (respectively, $\varphi_L(x)$, $\eta_L(x)$) equals -1 (respectively, $-L$, 0) if $x < -|L|$; 0 (respectively, x sign(L), sign(L)) if $-|L| < x < |L|$ and 1 (respectively, L, 0) if $x > |L|$. The complexity σ is found through maximising $-z^2/2 - w + \ln\lambda(z,w)$ over z, w and can in principle be computed for any α. The small α expansion of σ is computed from the expansion of ρ around the SK distribution $\rho^{\mathrm{SK}}(h_0,h_1) = \delta(h_0)\delta(h_1)$ using (13).

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