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Random free energies in spin glasses

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Résumé. — Les énergies libres des états purs sont étudiées dans la théorie de champ moyen. On montre qu'elles sont des variables aléatoires indépendantes avec une distribution exponentielle. Les implications sur les fluctuations avec les échantillons sont analysées. La nature physique de la théorie de champ moyen est complètement caractérisée.

Abstract. — The free energies of the pure states in the spin glass phase are studied in the mean field theory. They are shown to be independent random variables with an exponential distribution. Physical implications concerning the fluctuations from sample to sample are worked out. The physical nature of the mean field theory is fully characterized.

The physical understanding of the nature of the spin glass phase has improved recently with the detailed analysis of the solution proposed by one of us for the mean field theory of spin glasses introduced by Sherrington and Kirkpatrick (S.K.) [1]. It is known that the spin glass transition is associated with the breaking of ergodicity and the appearance of an infinite number of pure equilibrium states for the system, unrelated to each other by a symmetry. The spin glass phase can be understood by a geometrical analysis of the space of pure states. Each state α is characterized by its probability P_α, and the value of the local magnetization on each site $i : m_i^\alpha$. The order parameter [2] is the distribution of overlaps between two pure states α and β chosen with probabilities P_α and $P_\beta : P(q) = \sum_{\alpha,\beta} P_\alpha P_\beta \, \delta(q_{\alpha\beta} - q)$, where the overlap $q_{\alpha\beta}$ is equal to $(1/N) \sum_i m_i^\alpha m_i^\beta$.

It was further recognized in references [3, 4] that the probabilities of the states depend on the sample, and this was analysed [3] through the explicit computation of the inclusive distribution

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functions of the probabilities, $f^{(k)}$, defined as :

$$f^{(k)}(P_1, \ldots, P_k) = \overline{\sum_{\alpha_1 \ldots \alpha_k}' \delta(P_{\alpha_1} - P_1) \ldots \delta(P_{\alpha_k} - P_k)} \tag{1}$$

where the sum is carried over all couples of distinct replicas, and $\overline{(\ )}$ denotes the average over the realizations of the couplings.

In this paper we shall show that all these results on the distributions and fluctuations of the probabilities of the states are consequences of one simple property : *the free energies of the pure states are independent random variables.*

Let us make this statement more precise. All the pure states must have, in the thermodynamic limit, the same free energy per spin ($\lim_{N \to \infty} F_\alpha / N$). The probabilities of the different states are related to the $\mathcal{O}(1/N)$ corrections f_α/N to the free energy per spin by :

$$P_\alpha = \frac{e^{-\beta f_\alpha}}{\sum_\gamma e^{-\beta f_\gamma}} \tag{2}$$

(β is the inverse of the temperature). We shall prove that, within the solution of the S.K. model proposed in [5], the f_α are independent random variables with an exponential distribution :

$$\mathcal{T}_\rho(f_\alpha) = \rho . \exp \rho(f_\alpha - f_c) . \theta(f_c - f_\alpha) , \tag{3}$$

ρ is a function of the temperature and the external field H and is equal to $\beta(1 - y)$ where y is the width of the right plateau in $q(x)$, $y = \overline{\sum_\alpha P_\alpha^2}$; f_c is a cut-off free energy needed at an intermediate stage. We consider a finite number M of pure states with the distribution $\mathcal{T}_\rho$. In the end we send the cut-off f_c and M to infinity, while keeping a density of levels at any finite free energy fixed :

$$M \, e^{-\rho f_c} = v , \quad \begin{matrix} M \to \infty \\ f_c \to \infty \end{matrix} . \tag{4}$$

All our results are v independent.

In order to prove equation (3), we have computed within this model the inclusive distributions of the probabilities $f^{(k)}$ defined in (1), and verified that the results agree with those of the replica method given in [3]. We shall hereafter sketch the computation of the average number of states of a given probability $f^{(1)}(P)$.

From the relation (2) between the probabilities and the free energies, the expression of the kth moment M_k of $f^{(1)}(P)$ is :

$$M_k = \overline{\sum_\alpha P_\alpha^k} = M \int \prod_{\alpha=1}^{M} (\mathcal{T}_\rho(f_\alpha) \, df_\alpha) \, e^{-\beta k f_1} \left[\sum_{\gamma=1}^{M} e^{-\beta f_\gamma} \right]^{-k} . \tag{5}$$

Using an integral representation of the last term :

$$Z^{-k} = \frac{1}{\Gamma(k)} \int_0^\infty d\lambda \, \lambda^{k-1} \, e^{-\lambda Z} \tag{6}$$

we obtain :

$$M_k = M \int_0^\infty \mathrm{d}\lambda \frac{1}{\Gamma(k)} \lambda^{k-1} g(\lambda, k) [g(\lambda, 0)]^{M-1}$$

$$g(\lambda, k) = \int \mathcal{T}_\rho(f) \, \mathrm{d}f \exp[-\beta k f - \lambda \, \mathrm{e}^{-\beta f}]. \tag{7}$$

For $k > 0$ one gets in the limit $f_c \to \infty$:

$$g(\lambda, k) = \frac{\rho}{\beta} \mathrm{e}^{-\rho L} \lambda^{-k+\rho/\beta} \Gamma(k - \rho/\beta) \tag{8}$$

while for $k = 0$, the limit must be taken more carefully and gives (for $\rho < \beta$) :

$$g(\lambda, 0)^M \simeq \exp(-v\lambda^{\rho/\beta} \Gamma(1 - \rho/\beta)). \tag{9}$$

The value of M_k obtained from equations (7) to (9) is :

$$M_k = \Gamma(k - \rho/\beta) [\Gamma(k) \Gamma(1 - \rho/\beta)]^{-1} \tag{10}$$

which is exactly the kth moment of $f^{(1)}(P)$ given in [3] with the identification : $\rho/\beta = 1 - y$.

The general inclusive distribution $f^{(k)}$ can be computed in the same way. Alternatively one can use the following formula which we have obtained from equations (2) to (4) for the exclusive distribution f^{E} of all the probabilities :

$$f^{\mathrm{E}}(P_1, ..., P_M) = \frac{1}{M}(1 - y)^{M-1} \delta\left(1 - \sum_{k=1}^{M} P_k\right) P_{\min}^{M(1-y)} \prod_{k=1}^{M} P_k^{-2+y} \tag{11}$$

where $P_{\min}$ is the smallest P_k.

Thus the distribution of probabilities and the fluctuations from sample to sample reflect a simple random process : in each sample the probabilities are chosen according to equations (2) to (4). The dominance of certain states is associated to the finite probabilities of having finite gaps between the lowest levels. Finally we mention that the exponential distribution and the independence of the free energies can be understood more clearly on the « simplest spin glass model » [6], since this model is thermodynamically equivalent to a random (free-) energy model [7]. This model can be studied directly and leads to (3) and (4) with $v = 1/\rho = 1/(2\sqrt{\ln 2})$.

We shall now turn to the generalization of these results for the distribution of clusters of states, and deduce from it the fluctuations of the order parameter function.

Because of ultrametricity one can group together states which have a mutual overlap larger than a given value q, and this defines a partition of the states into nonoverlapping clusters [3]. The weight W_{I} of a cluster I being defined as the sum of the probabilities of the states it contains, it was shown in [3] that the inclusive distribution of weights at any scale have the same form as the distribution of probabilities of the states, but for a change of the parameter $\underline{y = y(q_M)}$ into $y(q)$. (The function $y(q)$ is related to the average order parameter function $\overline{P(q)}$ by $y(q) = \int_q^1 \overline{P(q')} \, \mathrm{d}q'$).

Hence the previous results also apply to the weights of the clusters. Defining for each cluster I at the scale q its generalized free energy $f_{\rm I}$ according to :

$$W_{\rm I} = \frac{e^{-\beta f_{\rm I}}}{\sum_{\rm I'} e^{-\beta f_{\rm I'}}} \tag{12}$$

the $f_{\rm I}$ are independent random variables with an exponential distribution as in equations (2) to (4), but with a value of ρ :

$$\rho(q) = \beta(1 - y(q)) . \tag{13}$$

Considering one cluster at the scale q_1 and its subclusters at the scale $q_2 > q_1$, we have found that the distribution of the free energies $f_1, ..., f_M$ of the M subclusters (M is finite if one imposes a cut-off f_c in free energy, and diverges as in (4) when $f_c \to \infty$) is :

$$\mathcal{T}_{q_1,q_2}(f_1, ..., f_M) = C\mathcal{T}_{\rho(q_2)}(f_1) \cdots \mathcal{T}_{\rho(q_2)}(f_M) \times [e^{-\beta f_1} + \cdots + e^{-\beta f_M}]^{\rho(q_1)/\beta} . \tag{14}$$

It is easy to generalize this equation to n clusters at scales $q_1, ..., q_n$.

These results allow for a clear understanding of some statements which appeared before in the literature :

— The universality property [3] : the whole dependence on the temperature, the magnetic field and the choice of the overlap is through a function $\rho_{T,H}(q)$, which is related to the average order parameter through equation (13).

— The content of the PaT approximation [8] from this perspective is that $\rho_{T,H}$ for $H = 0$ does not depend on T. The validity at low temperatures, verified in [9], reflects the fact that $\rho_{T,0}(q)$ has a limit $\rho_{0,0}(q)$, and does not depart too quickly from it at small T.

— Following reference [10] one can consider the states at a given value of T, H and weight them with a factor different from the Boltzmann factor, of the form :

$$P_\alpha^{(u)} = \frac{e^{-\beta u f_\alpha}}{\sum_\gamma e^{-\beta u f_\gamma}} . \tag{15}$$

As $\rho_{T,H}(q)$ and u appear in the formulae only in the ratio $\rho_{T,H}/(\beta u)$, one clearly finds in this case a new average order parameter $y^{(u)}(q)$ related to the normal one by (see Eq. (13)) :

$$1 - y^{(u)}(q) = \frac{1 - y(q)}{u} , \tag{16}$$

in agreement with the result of reference [10]. This different weighting of the states is possible when $\rho_{T,H}(q) < \beta u$ for all q, so that necessarily $u > u_c = 1 - y(q)$, which explains the existence of the critical value of u states in [10], and gives its explicit value.

We now turn to the computation of the fluctuations of the order parameter function. Following [3], we define for each sample a function $P_J(q)$ which depends on the particular realization of the couplings, and the integrated probability :

$$Y_J(q) = \int_q^1 P_J(q') \, dq' . \tag{17}$$

Calling I the clusters at the scale q and $W_{\rm I}$ their weights, one has simply $Y_J(q) = \sum_{\rm I} W_{\rm I}^2$, whose probability distribution $\Pi(Y)$ can be inferred from the exclusive distribution f^{E} of the weights (11), with $\rho = \beta(1 - y(q))$.

We introduce the auxiliary function $\hat{f}^{\mathrm{E}}(v, W_1, \ldots, W_M)$ which differs from f^{E} only by the fact that the sum $\sum_{i=1}^{M} W_i$ is constrained to be equal to v rather than 1 and we define the characteristic function $F_v(z)$:

$$F_v(z) = \int \mathrm{d}W_1 \ldots \mathrm{d}W_M \, \hat{f}^{\mathrm{E}}(v, W_1, \ldots, W_M) \exp\left(- z \sum_{k=1}^{M} W_k^2 \right) \tag{18}$$

so that

$$F_1(z) = \int_0^1 \Pi(Y) \, \mathrm{e}^{-zY} \, \mathrm{d}Y \, . \tag{19}$$

The scaling relation $F_v(z) = F_1(zv^2)/v$, $v > 0$ allows one to write :

$$\int_0^\infty \frac{\mathrm{d}v}{v} \, \mathrm{e}^{\varepsilon v} \frac{\partial}{\partial z} F_1(zv^2) = \int_0^\infty \mathrm{d}v \, \mathrm{e}^{\varepsilon v} \frac{\partial}{\partial z} F_v(z) \tag{20}$$

where $\varepsilon = \pm 1$ and the $\partial/\partial z$ has been introduced to insure the convergence of the integrals at $v = 0$. This gives implicitly the characteristic function F_1 since the right hand side of equation (20) can be computed, and is equal to $\frac{1}{y-1} \frac{\partial}{\partial z} \log(H(z))$, where :

$$H(z) = \int_0^\infty \frac{\mathrm{d}P}{\Gamma(y)} P^{-1+y}(- \varepsilon + 2 zP) \, \mathrm{e}^{\varepsilon P - zP^2} \, . \tag{21}$$

We have used equations (20) and (21) in two different ways.

1) Taking $\varepsilon = -1$, integrating (20) for z between 0 and z_0, and expanding in powers of z_0, one finds the explicit formula for the moments of Π [11] :

$$\int_0^1 \Pi(Y) \, Y^p \, \mathrm{d}Y = \frac{1}{(y-1)} \frac{1}{(2p-1)!} \frac{\partial^p}{\partial t^p} \left[\mathrm{Log} \sum_{k=0}^{\infty} \frac{t^k}{k!} \frac{\Gamma(2k - 1 + y)}{\Gamma(-1 + y)} \right] \Bigg|_{t=0} \quad (p \geqslant 1) \tag{22}$$

which agrees with the diagrammatic expansion we gave in [3], and can be used to generate in a fast way a large number of moments.

2) Taking $\varepsilon = 1$ and changing variables in (20) from v to $v\sqrt{Y}$, one gets :

$$\int_0^\infty \mathrm{e}^{-zv} g(v) \, \mathrm{d}v = \frac{y}{z} \frac{D_{-1-y}(-1/\sqrt{2z})}{D_{+1-y}(-1/\sqrt{2z})} \tag{23}$$

with

$$g(v) = \int_0^1 \Pi(Y) \, \mathrm{e}^{\sqrt{v/Y}} \, \mathrm{d}Y \tag{24}$$

and where D_α are parabolic cylindric functions [12].

The singularity of $\Pi(Y)$ at $Y = 0$ is given by the behaviour of $g(v)$ for $v \to \infty$ which is itself (from Eq. (23)) dominated by the largest number z_0 such that $-1/\sqrt{2z_0}$ is a zero of D_{1-y}. Thus we find that $\Pi(Y)$ has an essential singularity at the origin :

$$\Pi(Y) \overset{Y \to 0}{\sim} \exp - [1/(4 z_0 Y)] . \tag{25}$$

This knowledge, together with the known divergence in $(1 - Y)^{-y}$ at $Y = 1$, and the formula (22) used to generate many moments, should allow a safe reconstruction of $\Pi(Y)$.

To conclude, we have shown that within the replica symmetry breaking ansatz proposed in [5], the free energies of the pure equilibrium states in the spin glass phase are independent random variables with an exponential distribution. Similar results are obtained for the cluster distributions. The physical content of the ansatz has now been found. Ultrametricity plus the properties investigated in this paper are not only consequences of the form of the ansatz but are equivalent in the sense that if they are assumed the form of replica symmetry breaking is determined.

Note added : After this work was completed we learned that our colleagues B. Derrida and G. Toulouse have independently obtained some results similar to ours on the fluctuations of the order parameter function.

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