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On chaos in mean-field spin glasses

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Abstract. We study the correlations between two equilibrium states of SK spin glasses at different temperatures or magnetic fields. The question, previously investigated by Kondor and Kondor and Végsö, is approached here by constraining two copies of the same system at different external parameters to have a fixed overlap. We find that imposing an overlap different from the minimal one implies an extensive cost in free energy. This confirms by a different method Kondor's finding that equilibrium states corresponding to different values of the external parameters are completely uncorrelated. We also consider the generalized random energy model of Derrida as an example of a system with strong correlations between states at different temperatures.

1. *Introduction*

The structure of the equilibrium states of mean-field spin glasses has been widely discussed in the literature [1]. At low temperature ergodicity is broken, and the contribution to the Boltzmann average comes from 'valleys' separated by infinite barriers. The statistics of the correlations between the different valleys for equal values of the external parameters is one of the most remarkable outcomes of the replica method. In the context of the Parisi ansatz, it is found that the function $q(x)$ is directly related to the statistics of couples of valleys, while the whole set of states is organized as an ultrametric tree. Much less information is available about the relations between the equilibrium states for different values of the external parameters. The object of this paper is an investigation of this relation.

The states of mean-field spin glasses can be thought as a low-free-energy solution of the TAP equations. Changes in the external parameters can cause the appearance or the disappearance of solutions and modify the relative order of the free-energy levels. There are models, for example the p-spin spherical spin glass, where the order of the levels is not affected by changes in temperature [2]. In this case the states at different temperatures are correlated.

In a model where a change in an external parameter implies a reshuffling of the states *by an extensive amount*, one can expect that the low-lying states at a given value of the parameter will become highly excited states as the parameter is changed. For entropic

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reasons one would then find zero correlations between the new and the old equilibrium states.

The first suggestions that states in the SK model corresponding to different external parameters could be uncorrelated date back to Parisi in the case of magnetic field [3] and to Sompolinsky [4] in the case of temperature. The problem has been addressed analytically by Kondor [5] and Kondor and Végsö [6]. Within the frame of the replica method they considered the partition function of two realizations of the same system for different external parameters. In these papers constant correlations were assumed; this constant was found to be zero in mean field and the Gaussian corrections to this situation were computed.

Here we re-examine the question without using this assumption. Instead we follow a method introduced in [7], and we take into account in the partition function (Z) of the two systems only these couples of configurations having overlap equal to a fixed value p_d. It was shown in [7], in the case of two systems at equal external parameters, that if p_d is in the support of the probability function $P(q)$, the logarithm of the constrained partition function is extensively equal to that of an unconstrained system. This result tells us simply that the partition function is dominated by these couples of equilibrium states which satisfy the constraint. Conversely, if p_d is out of the support of the $P(q)$ the system is forced out of equilibrium and this implies an extensive increase of the free energy $F = -\log Z$.

In the present case, an extensive increase in F implies a reshuffling of the free-energy level of an extensive amount, and zero correlation between states for different external parameters. The method, relying on the saddle-point approximation, is limited to the computation of the extensive part of the free energy. So, a zero cost in free-energy density would not strictly imply no reshuffling, but just that the reshuffling is not extensive. With reference to the theory of dynamical systems, the situations in which small control parameter changes imply uncorrelated equilibrium states has been often referred to as 'chaotic'. We will use this term in a more restrictive way to denote a situation where the free-energy increase resulting from the imposition of a fixed overlap $p_d \neq 0$ is extensive.

The paper is organized as follows. In section 2 we state the basic definitions and our method. In section 3 we discuss the problem in the simple case of the Derrida generalized random energy model (GREM), where handwaving arguments show that there is no chaos with temperature in absence of a magnetic field, and along the lines of constant magnetization. We show how some modifications in those models produce chaos with temperature. In section 4 we study the SK model near the glassy transition. We show that no ultrametric solution exists for the problems with different magnetic fields or temperatures. We argue that this is the sign that chaos is present in both cases and give estimation for the free-energy increase. Finally we draw our conclusions in section 5.

2. The model

Let us consider a system composed of two copies of a Sherrington Kirkpatrick (SK) model, having different temperatures and magnetic fields (T_1, h_1) and (T_2, h_2), respectively. The partition function of such a system is

$$Z = \sum_{\{S_i^1, S_i^2\}} \exp\left[\beta_1 \sum_{i<j}^{1,N} J_{ij} S_i^1 S_j^1 + h_1 \sum_{i}^{1,N} S_i^1 + \beta_2 \sum_{i<j}^{1,N} J_{ij} S_i^2 S_j^2 + h_2 \sum_{i}^{1,N} S_i^2\right] = Z_1 Z_2 \qquad (1)$$

where the couplings J_{ij} $(i, j = 1, \ldots, N)$ are Gaussian independent variables of zero mean and variance $1/N$, and the spins S_i^r are Ising variables. In what follows we will improperly call *free energy* the quantity $F = -\log Z$. To address the question of the correlations between the states dominating Z_1 and Z_2, respectively, let us consider $Z(p_d)$ the sum (1) restricted to those configurations which satisfy

$$p_d = \frac{1}{N}\sum_i S_i^1 S_i^2. \tag{2}$$

It is clear from the definition that $Z(p_d) \leqslant Z$. It is shown in [7] in the case $T_1 = T_2$ and $h_1 = h_2$ that, in the low-temperature phase, one has $(1/N)\log Z = (1/N)\log Z(p_d)$ as soon as p_d is in the support of the function $P(q)$ of the free system. This is a consequence of the fact that the number of valleys dominating the partition function grows less then exponentially with N, as can easily be understood noting that $Z = \int \mathrm{d}p_d Z(p_d)$. An increase in free energy at an extensive level implies the absence of low-lying states having overlap p_d.

In [7] it was shown how to deal with a problem of two coupled copies with the replica method. We shall not repeat the derivation of formulae that are completely analogous to those in [7] here, but we shall just sketch the results. Instead of the usual order parameter matrix Q_{ab} of the replica method, there are three matrices $Q_{ab}^{(1)}$, $Q_{ab}^{(2)}$ and P_{ab} representing respectively

$$Q_{ab}^{(r)} = \frac{1}{N}\sum_{i=1}^{N} S_i^{ra} S_i^{rb} \quad r = 1, 2 \qquad P_{ab} = \frac{1}{N}\sum_{i=1}^{N} S_i^{1a} S_i^{2b} \tag{3}$$

where $a, b = 1, \dots, n$ and n is 'the number of replicas', which as usual has to be sent to zero. The constraint in the partition function implies that the elements P_{aa} have to be set equal to p_d. Combining $Q^{(1)}$, $Q^{(2)}$, P and its transpose P^{T} into the matrix

$$\mathbf{Q} = \begin{pmatrix} Q^{(1)} & P \\ P^{\mathrm{T}} & Q^{(2)} \end{pmatrix}$$

and denoting its elements by $\mathbf{Q}_{\alpha\beta}$, $\alpha = (r, a)$, $\beta = (s, b)$, it is possible to see, for both T_1 and T_2 near the critical temperature $T_c = 1$ and h_1 and h_2 small, that $\mathbf{Q}_{\alpha\beta} \sim 1 - T_1$ and the free energy admits the expansion up to fourth order in $T_s - T_c$ ($s = 1, 2$):

$$\begin{aligned} F(p_d) &= -\lim_{N\to\infty} \frac{1}{N}\log Z(p_d) \\ &= -\lim_{n\to 0}\frac{1}{2n}\Big\{\tau_1 \operatorname{Tr} Q^{(1)2} + \tau_2 \operatorname{Tr} Q^{(2)2} + 2\tau_{12}\operatorname{Tr} P^2 + \frac{w}{3}\operatorname{Tr}\mathbf{Q}^3 \\ &\quad + \frac{u}{6}\sum_{\alpha\beta}\mathbf{Q}_{\alpha\beta}^4 + \frac{v}{4}\operatorname{Tr}\mathbf{Q}^4 - \frac{y}{2}\sum_{\alpha\beta\gamma}\mathbf{Q}_{\alpha\beta}^2\mathbf{Q}_{\beta\gamma}^2 \\ &\quad + h_1^2\sum_{ab} Q_{ab}^{(1)} + h_2^2 \sum_{ab} Q_{ab}^{(2)} + 2h_1 h_2 \sum_{ab} P_{ab}\Big\} \end{aligned} \tag{4}$$

where

$$\tau_s = (1 - T_s^2)/2 \quad s = 1, 2 \qquad \tau_{12} = (1 - T_1 T_2)/2. \tag{5}$$

For the 'complete' SK model $y = u = v = w = 1$. It is customary in the study of the glassy transition to consider a 'truncated' (or 'reduced') model in which it is artificially posed that $y = v = 0$, and in which only the term $\sum_{\alpha\beta}\mathbf{Q}_{\alpha\beta}^4$ is retained from among all the quartic terms. Kondor and Végsö have shown recently that this can give rise to instabilities in considering couples of systems with different temperatures when the magnetic field is zero. We anticipate that the arguments showing the presence of chaos do not depend critically on which of the two models is used. So, we will use the complete model to prove the presence of chaos and we will estimate the free-energy increase within the truncated one. In any case, equation (4) has to be maximized with respect to the values of the elements of the replica matrices.

The basic object of our investigation will be the free-energy difference

$$\Delta F = F(p_d) - F \tag{6}$$

where F is the logarithm of the partition function of the two systems (at two different external parameters) without constraint, and is equal to the sum of the free energies of the two systems. In what follows we will refer to ΔF as 'free-energy excess', and to 'chaos' whenever this quantity is non-zero.

Following [7] we will consider here an analytic continuation to $n \to 0$ for $F(p_d)$ in which each of the matrices $Q^{(r)}$ and P are parametrized according to the Parisi scheme, that is, specifying the value of the diagonal elements as a function of the interval [0,1] according to

$$Q^{(r)} \to (0, q_r(x)) \qquad P \to (p_d, p(x)) \qquad 0 \leqslant x \leqslant 1. \tag{7}$$

The usual restriction of the choice of the Parisi function to the space of non-decreasing function is substituted here by the requirement of semi-positive definiteness of the matrices

$$\begin{pmatrix} q_1'(x) & p'(x) \\ p'(x) & q_2'(x) \end{pmatrix} \tag{8}$$

for any x, where the primes denote differentiation with respect to x [8]. In particular, this implies that the functions $q_s'(x)$ are both positive.

The saddle-point equations for the maximization of $F_2(p_d)$ of the truncated model are written in terms of the $q_s(x)$ and $p(x)$ as

$$\begin{aligned}\frac{\delta F}{\delta q_s(x)} &= 2[\tau_s - \langle q_s\rangle]q_s(x) + 2[p_d - \langle p\rangle]p(x) - \int_0^x \mathrm{d}y\, [q_s(x) - q_s(y)]^2 \\ &\quad - \int_0^x \mathrm{d}y\, [p(x) - p(y)]^2 + \tfrac{2}{3}q_s^3(x) + h_s^2 = 0\end{aligned} \tag{9}$$

$$\begin{aligned}\frac{\delta F}{\delta p(x)} &= [\tau_{12} - \langle q_1 + q_2\rangle]p(x) + [p_d - \langle p\rangle][q_1(x) + q_2(x)] \\ &\quad - \int_0^x \mathrm{d}y\, [q_1(x) - q_1(y) + q_2(x) - q_2(y)][p(x) - p(y)] \\ &\quad + \tfrac{2}{3}p^3(x) + h_1 h_2 = 0.\end{aligned} \tag{10}$$

We also write for future reference the expression for the derivative of F with respect to p_d:

$$\frac{\partial F}{\partial p_d} = -\big[\tau_{12}p_d - \langle p(q_1 + q_2)\rangle + \tfrac{2}{3}p_d^3 + h_1 h_2\big]. \tag{11}$$

Our variational equations differ from the one considered in [5, 6] in the fact that there p_d was taken as a variational parameter and the function $p(x)$ was constrained to a constant. We will see in the next section that models without chaos require non-constant $p(x)$.

Before starting to discuss the maximization of (4) and the solutions of (9), (10), we discuss the correlations between states at different temperature and magnetic field in the GREM.

3. The GREM: a model without chaos

Let us briefly review Derrida's construction of the generalized random energy model. Without any pretension of being exhaustive on this point, we refer the reader to the original papers on the model [9–11].

In the GREM one considers 2^N configurations, associated with the 'leaves' of an ultrametric tree. The tree is composed of L levels of branching. At a level α, each branch generates $\mathcal{N}_\alpha = \exp(NS_\alpha)$ new branches, in such a way that $2^N = e^{N\sum_\alpha S_\alpha}$. A random energy is associated with each branch at a level α, so that the total energy of a configuration is given by $E = \sum_\alpha \epsilon_\alpha$. The ϵ_α are taken as independent Gaussian variables of zero mean and variance $\overline{\epsilon_\alpha^2} = NJ_\alpha^2/2$. Two configurations are conventionally said to have an overlap q_α, with $0 \leqslant q_\alpha \leqslant 1$, if they coincide at a level α, and consequently have the same ϵ_β for $\beta \leqslant \alpha$. It can eventually be considered as a 'continuum limit' of infinite number of levels $(L \to \infty)$ with infinitesimal spacings, where $J_\alpha \to J(q)\mathrm{d}q$, $S_\alpha \to S(q)\mathrm{d}q$. This exhausts the construction in the absence of a magnetic field. In the presence of a magnetic field h one has to associate magnetization one with an arbitrarily selected state, in such a way that the configurations of magnetization m are those having an overlap equal to m with this state. For these states the energy gets an extra contribution equal to $-Nhm$, where h is the magnetic field.

In what follows we will limit our discussion to the case where $J(q)$ and $S(q)$ increase with q, where the levels associated with small q freeze at a higher temperature than the levels of high q.

The absence of chaos with varying temperature in zero magnetic field is almost obvious; by definition of the model, a change in temperature does not affect the order of the energy levels. So, two equilibrium states at different temperatures T and T' can be strongly correlated. In the same way it is easy to realize that there is chaos with the magnetic field. Two different magnetic fields, say h_1 and h_2, impose respective magnetizations m_1 and m_2 on the system, with $m_1 \neq m_2$. By construction the overlap between two states with such different magnetizations is equal to $q_{12} = \min\{m_1, m_2\}$. Imposing a different overlap would bring the magnetizations out of their equilibrium values, implying an extensive cost in terms of free energy. Furthermore, in the presence of a magnetic field, a change in temperature implies a change in the magnetization, and again we find chaos. Thus chaos is clearly absent along the lines (T, h) of constant magnetization†.

Let us now show with the aid of the replica method that, for two different temperatures in zero magnetic field, there is no free-energy cost in imposing an overlap p_d in the support of the function $P(q)$. Note that the same results could easily be obtained with the Derrida probabilistic technique. The replicated partition function of the GREM in zero field, in the discrete formalism, is

$$\overline{Z^n} = \overline{\sum_{\{j_{a,s}^\alpha\}} \exp\left(-\sum_{s,a,\alpha} \beta_s \epsilon_{j_{a,s}^\alpha}\right)} \prod_{\alpha\leqslant\alpha_0} \delta_{j_{a,1}^\alpha, j_{a,2}^\alpha} \tag{12}$$

where the level α_0 corresponds to the overlap p_d, $\alpha = 1, \ldots, L$, $s = 1, 2$ and $a = 1, \ldots, n$ is the replica index. On performing the average over the values of the energy levels one gets

$$\overline{Z^n} = \sum_{\{j_{a,s}^\alpha\}} \exp\left(\frac{N}{4}\sum_{\alpha,r,s} J_\alpha^2 \beta_r \beta_s \sum_{ab} \delta_{j_{a,r}^\alpha, j_{b,s}^\alpha}\right) \prod_{\alpha\leqslant\alpha_0} \delta_{j_{a,1}^\alpha, j_{a,2}^\alpha}. \tag{13}$$

† We thank J Kurchan for this observation.

To evaluate the partition function we make the following ansatz on the arrangement of the replicas. We suppose that for the levels $\alpha \leqslant \alpha_0$, where $j^\alpha_{a,1} = j^\alpha_{a,2}$, the replicas are divided into n/x_α groups of x_α coinciding states (i.e. $j^\alpha_{a,r} = j^\alpha_{b,s}$ for any r, s if a and b are in the same group). For the levels $\alpha \geqslant \alpha_0$, one has $j^\alpha_{a,1} \neq j^\alpha_{a,2}$, and one can divide, accordingly to the same scheme the replicas with $s = 1$ and $s = 2$ into n/x^1_α and n/x^2_α groups, respectively. It is easy to see that the free energy is given by the expression

$$\frac{1}{nN}\log\overline{Z^n} = \sum_{\alpha\leqslant\alpha_0}\left[\frac{S_\alpha}{x_\alpha} + (\beta_1+\beta_2)^2 J^2_\alpha x_\alpha\right] + \sum_{\alpha>\alpha_0}\left[S_\alpha\left(\frac{1}{x^1_\alpha}+\frac{1}{x^2_\alpha}\right) + J^2_\alpha(\beta^2_1 x^1_\alpha + \beta^2_2 x^2_\alpha)\right] \tag{14}$$

taken at the saddle point over the various x. Assuming that the level α_0 is frozen at the temperatures T_1 and T_2, one finds, on differentiating with respect to x_α, x^1_α and x^2_α, that

$$\begin{cases} (\beta_1+\beta_2)^2 x^{s\,2}_\alpha = \dfrac{S_\alpha}{J^2_\alpha} & \alpha \leqslant \alpha_0 \\ \beta^2_s x^{s\,2}_\alpha = \dfrac{S_\alpha}{J^2_\alpha} & \alpha > \alpha_0 \text{ and } S_\alpha/(J^2_\alpha\beta^2_s) < 1 \\ x^s_\alpha = 1 & \alpha > \alpha_0 \text{ and } S_\alpha/(J^2_\alpha\beta^2_s) > 1. \end{cases} \tag{15}$$

Substituting these in (14) one sees easily that $(1/N)\log\overline{Z^n} = (1/N)[\log\overline{Z^n_1} + \log\overline{Z^n_2}]$, that is, we find no chaos with temperature.

It is interesting to note that, in the continuum limit, inverting the functions $x(q)$ and $x_s(q)$, the functions $q_s(x)$ and $p(x)$ take the form:

$$q_s(x) = \begin{cases} q_u((\beta_1+\beta_2)x) & x \leqslant x_0 \\ p_d & x_0 \leqslant x \leqslant x_s \\ q_u(\beta_s x) & x > x_s \end{cases} \tag{16}$$

$$p(x) = \begin{cases} q_u((\beta_1+\beta_2)x) & x \leqslant x_0 \\ p_d & x_0 \leqslant x \end{cases} \tag{17}$$

where $q_u(\beta x)$ is the inverse function of $\beta x(q) = S(q)/J^2(q)$, and the points x_0 and x_s are defined by the relations

$$q_u((\beta_1+\beta_2)x_0) = q_u(\beta_s x_s) = p_d. \tag{18}$$

The only solution with a constant $p(x)$ is the one with $p_d = p(x) = 0$.

So we have shown, in a situation where the order of the levels does not depend on the temperature, that imposing an overlap p_d in a suitable interval does not imply an extensive free-energy cost, i.e. chaos with does not occur with temperature. The situation is different if the ordering of the state depends on the temperature. In the context of the GREM, such a dependence can be introduced upon considering one or two of the following modifications:

- choosing temperature dependent S_α or J_α;
- not imposing the identity of the levels for different temperatures.

This can be done without dramatically changing the organization of the states at fixed temperature and the temperature dependence of the free energy. Here we choose to discuss the simplest case, namely the second possible modification. We take a REM (i.e. a GREM with only one level, $L = 1$), where the Gaussian energies depend on T, and the correlations are specified by

$$\overline{\epsilon_j(T_1)\epsilon_k(T_2)} = \delta_{j,k}\tfrac{1}{2}C(T_1, T_2)N \tag{19}$$

where $C(T_1, T_2) \leqslant J^2 = C(T, T)$. The model can easily be analysed with the probabilistic method used by Derrida to solve the REM. For the sake of brevity, we give our results in the frame of the replica method. Let us compute the free energy of two replicas, at temperatures T_1 and T_2 below the freezing transition, constrained to be in the same state

$$\begin{aligned}\overline{Z^n} &= \sum_{j^a} \overline{\exp\left[-\beta_1\epsilon_j^a(T_1) - \beta_2\epsilon_j^a(T_2)\right]} \\ &= \sum_{j^a} \exp\left\{N\left[(\beta_1^2 + \beta_2^2)J^2 + 2\beta_1\beta_2 C(T_1, T_2)\right]\sum_{ab}\delta_{j^a,j^b}\right\}.\end{aligned} \tag{20}$$

Proceeding as above for the GREM (dividing the replicas into groups), one finds that

$$\frac{1}{nN}\log\overline{Z^n} = \sqrt{\log 2((\beta_1^2 + \beta_2^2)J^2 + 2\beta_1\beta_2 C(T_1, T_2))} \leqslant \frac{1}{nN}\log\overline{Z_1^n} + \frac{1}{nN}\log\overline{Z_2^n}. \tag{21}$$

The equality is recovered for $C(T_1, T_2) = J^2$ which corresponds to identical levels at the two temperatures. It would be interesting to understand if this mechanism which produce chaos with temperature is of any relevance in microscopic models.

4. Chaos in the SK model

Let us now turn to the study of the SK model and investigate the possibility of an absence of chaos. A possible scenario implying the absence of chaos has been proposed in [12]. The states at different temperatures are strongly correlated. On lowering the temperature the ultrametric tree of states undergoes multifuractions in such a way that the states at the *new temperature are the descendents in the tree of the ones at the old temperature.* This is what happens in the GREM, and it seems reasonable that whenever chaos is absent this must be the correct picture: the states at different temperatures must be part of the same ultrametric tree. In this case the total matrix $\mathbf{Q}_{\alpha\beta}$ should be ultrametric: for any given three distinct replicas α, β, γ one should find $\mathbf{Q}_{\alpha\beta} \geqslant \min\{\mathbf{Q}_{\alpha\gamma}, \mathbf{Q}_{\beta\gamma}\}$. Specializing the relation to $\alpha = (1, a)$, $\beta = (2, a)$, $\gamma = (1, c)$, that is, $Q_{1a,2a} = P_{aa} = p_d$, it is easily found that

$$Q_{1c,2a} = P_{ac} = \begin{cases} p_d & Q_{1a,1c} \geqslant p_d \\ Q_{1a,1c} & Q_{1a,1c} < p_d. \end{cases} \tag{22}$$

If we suppose that, as in the case of coinciding external parameters, the functions $q_s(x)$ and $p(x)$ are continuous [7], we find that condition (22) reflects on the functions $q_s(x)$ and $p(x)$ in the following way: $q_1(x)$ and $q_2(x)$ must be non-decreasing in the whole interval [0, 1], and a point $\overline{x}$ in [0,1] must exist such that

$$\begin{aligned} &q_s(x) = p(x) = q_<(x) \qquad x \leqslant \overline{x} \\ &p(x) = p_d \qquad x > \overline{x}. \end{aligned} \tag{23}$$

By continuity one has $q_<(\overline{x}) = p_d$.

The solution (16), (17) for the GREM is obviously of the form proposed here. A solution of this form was found in [7] in the case where $T_1 = T_2 = T$ and $h_1 = h_2 = h$. It reads

$$q_1(x) = q_2(x) = \begin{cases} q_F(2x) & 0 \leqslant x \leqslant x_0/2 \\ p_d & x_0/2 \leqslant x \leqslant x_0 \\ q_F(x) & x_0 \leqslant x \leqslant 1 \end{cases} \tag{24}$$

$$p(x) = \begin{cases} q_F(2x) & 0 \leqslant x \leqslant x_0/2 \\ p_d & x_0/2 \leqslant x \leqslant 1 \end{cases} \tag{25}$$

where the function $q_F(x)$ is the 'free' Parisi function

$$q_F(x) = \begin{cases} q_{\min} = \left(\dfrac{3h^2}{4}\right)^{\frac{1}{3}} & 0 \leqslant x \leqslant x_{\min} \\ \dfrac{x}{2} & x_{\min} \leqslant x \leqslant x_{\max} \\ q_{\max} = \dfrac{1-\sqrt{1-4\tau}}{2} & x_{\max} \leqslant x \leqslant 1 \end{cases} \tag{26}$$

in which x_0 is the point defined by $q_F(x_0) = p_d$, and $x_{\min}$ and $x_{\max}$ are given by continuity. The interval of p_d for which this solution is well defined, and that will be considered in what follows, is $q_{\min} \leqslant p_d \leqslant q_{\max}$. The form (24), (25) is not limited to this problem; simply as a consequence of ultrametricity any model with replica symmetry breaking admits (24), (25) as solution of the two-replica problem if the function $q_F(x)$ solves the single-replica one [13].

The main result of this paper is that, as long as $T_1 \neq T_2$ or $h_1 \neq h_2$, an ultrametric solution of the kind (23) does *not* exist for either the truncated or complete models of section 2. A proof of this fact can be given assuming a form of the kind (23) and showing that it does not satisfy the saddle-point equations. We postpone this proof to the appendix; despite its conceptual simplicity the proof, already rather technical for the reduced model, is complicated by the necessity of using the complete model if we want full control over all the terms of order τ_1^4 in the free energy.

We conclude that chaos must be present both in temperature and magnetic field.

We shall now give some estimate for the free-energy excess when the constraint (2) is imposed in various situations. The solution of equations (9), (10) for generic values of temperature, magnetic field and p_d is very difficult to find. We have seen that the situation simplifies for $h_1 = h_2$ and $T_1 = T_2$ where the solution for generic p_d is (24)–(26). Other simple cases, to be presented below, are found for $T_1 \neq T_2$ and $h_1 \neq h_2$ for special values of $p_d \equiv p_d^0$ which permit functions $p(x)$ that are constant with x. It is easy to find that in this last case the system verifies $\partial F/\partial p_d = 0$, that is, the free energy is an extremum with respect to p_d. The only stable solution is the one which is a minimum with respect to p_d [5], and has a free-energy excess equal to zero†. It is easy to find that this solution must satisfy

$$q_s(x) = q_F(x) \qquad \text{and} \qquad p(x) = p_d. \tag{27}$$

The values of p_d for which this solution exists satisfy

$$\tau_{12} p_d - \langle q_1 + q_2 \rangle p_d + y p_d^3 + h_1 h_2 = 0 \tag{28}$$

† The reader should not be confused at this point; we are by no means extremizing F with respect to p_d, but we are claiming that a special value p_d^0 exists, for which the free energy has a stable saddle point with $p(x) = \text{constant}$.

which coincides with $\partial F/\partial p_d = 0$ (see equation (11)). This solution was first found by Kondor in [5]. It is the only solution we found which has zero free-energy excess and it implies minimal correlations between states corresponding to different parameters.

We shall use both the solutions (24), (25) and (27), (28) as starting points to compute the free-energy excess perturbatively in some small parameter. We shall consider the three following limiting situations:

- Case 1. $T_1 = T_2$, $h_1 \neq h_2$, $p_d = p_d^0 + \delta p_d$ and we perturb for small δp_d around the solution of (10) with $p(x) = p_d^0$.
- Case 2. $T_1 = T_2$, $h_2 = h_1 + \delta h$ fixed p_d and we perturb for small δh around the solution (24), (25).
- Case 3. $T_1 \neq T_2$, $h_1 = h_2$, $p_d = p_d^0 + \delta p_d$ and we solve perturbatively in δp_d.

In all cases, instead of solving equations (9), (10) even in an approximated form, we will suitably parametrize the functions $q_s(x)$ and $p(x)$, and maximize the free-energy functional with respect to these parameters. This variational procedure will enable us to obtain lower bounds for the free-energy excess in the various situations. We expect, however, to obtain the correct order of magnitude for ΔF as a function of the various external parameters. The whole program is analogous to the one pursued in [7] for computing the free-energy excess to have p_d out of the support of the $P(q)$ for identical parameters, or in [8] for studying violations of ultrametricity. We refer the interested reader to these papers for a more detailed presentation.

Let us illustrate case 1 as an example. For $p_d = p_d^0 + \delta p_d$ ($\delta p_d \ll p_d^0$) we look for functions $q_s(x)$ and $p(x)$ equal to (27) plus some small variations. These variations, that we call $\delta q_s(x)$ and $\delta p(x)$, have to be of order of δp_d in the saddle-point solution. We choose to parametrize them as follows:

$$
\begin{aligned}
\delta q_1(x) &= \begin{cases} \delta q_1^1 & x < x_m/2 \\ \delta q_1^2 & x_m/2 < x < x_1 + \delta x_1 \\ 0 & x > x_1 + \delta x_1 \end{cases} \\
\delta q_2(x) &= \begin{cases} \delta q_2^1 & x < x_m/2 \\ \delta q_2^2 & x_m/2 < x < x_2 + \delta x_2 \\ 0 & x > x_2 + \delta x_2 \end{cases} \\
\delta p(x) &= \begin{cases} \delta p^1 & x < x_m/2 \\ \delta p^2 & x > x_m/2 \end{cases}
\end{aligned}
\tag{29}
$$

where $x_m/2$ is arbitrarily chosen as the middle of the first plateau in q_F, i.e. $x_m = \min[x_1, x_2]$ with $x_s = 2q_{\min}^s$ and $q_{\min}^s = (3h_s^2/4)^{1/3}$, $(s = 1, 2)$. The various parameters appearing above are determined by maximization of the free-energy functional supposing self-consistently that they are of order δp_d. It turns out that to lowest order the free-energy excess is of order δp_d^2. As we are only interested in lowest-order terms, we can minimize the polynomial of order two thus obtained by expanding up to second order the free-energy functional in all the parameter of order δp_d^2. The resulting saddle-point equations are linear equations in the (10) variational parameters, that we solved numerically for given values of τ, h_1 and h_2. In figure 1 we present the result for the free-energy excess at some values of the external parameters. We also solved analytically the equations in the two limit cases: (i) $h_2 = 0$ and (ii) $h_2 = h_1 + \delta h$ with $\delta h \ll h_1$. In this last case we just computed ΔF to the first order

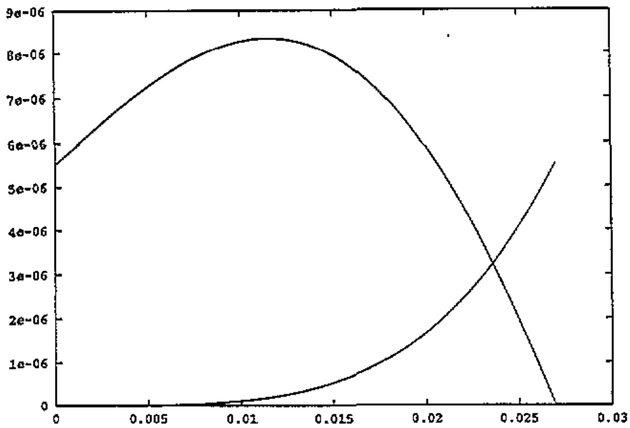

Figure 1. The free-energy excess $\Delta F/\delta p_d^2$ as a function of $q_{\min}^2 = \left(\frac{3}{4}h_2^2\right)^{1/3}$ in two cases. Upper curve: $q_{\min}^1 = 0.027$, $h_1 = 0.0038$, $\Delta F = 0$ for $q_{\min}^2 = 0.027$. Lower curve: $q_{\min}^1 = h_1 = 0$ $\Delta F = 0$ for $q_{\min}^2 = 0$. The symmetry of ΔF as a function of q_1 and q_2 implies that two curves are equal in the opposite extremes.

in δh. The results for these two cases are:

$$\Delta F = \begin{cases} \left(\dfrac{2187}{32}\right)^{1/3} \delta p_d^2\, h_1^{8/3}/q_{\max} & h_2 = 0 \\ \dfrac{1}{\sqrt{2}}\delta p_d^2\, h_1\, \delta h & \delta h \ll h_1. \end{cases} \tag{30}$$

In all cases the variational parameters turned out to be consistent with the hypothesis of being of order δp_d and with the positivity condition (8), e.g. in the case $h_2 = 0$, $h_1 \neq 0$, $x_m = 0$, we found $\delta q_1^2 = -\delta p_d q_{\min}/(4q_{\max} - 3q_{\min})$ and $\delta p^1 = \delta p^2 = \delta p_d$, the other variables being zero.

The computation of case 2 for small field difference $\delta h = h_2 - h_1$ follows a very similar scheme. In this case we perturb around the solution of the problem with $\delta h = 0$ (24), (25) with $q_{\min} \leqslant p_d \leqslant q_{\max}$. Without entering in the details of the solution, which is similar to the one of the previous case, we give the result. Under the (self-consistent) hypothesis that all the variations are of order δh one finds that the free-energy excess is of order δh^2. We get

$$\Delta F = \tfrac{2}{3}\delta h^2 (p_d - q_{\min})(p_d + q_{\min}) \frac{(3p_d^2 + 3p_d q_{\min} + 2q_{\min}^2)}{p_d^2 + p_d q_{\min} + 2q_{\min}^2}. \tag{31}$$

Note that the free-energy excess is zero for $p_d = q_{\min}$, as it should be.

Very similar paths can be followed to study the case 3 of chaos with temperature. Here we found for the free-energy excess:

$$\Delta F = \delta p_d^2 \frac{(T_1 - T_2)^4}{\tau_1}. \tag{32}$$

It is worth noting that equation (32) is derived from the truncated model in a magnetic field $h_1 = h_2 = h$ but does not depend on h. As was noted by Kondor and Végsö [6], the truncated model presents a spurious instability in the fluctuation matrix. The result (32) shows that our calculation is insensitive to this instability.

Equations (30)–(32) can be used to estimate the probability distribution for an overlap p_d between states at different parameters in finite systems via the relation $\mathcal{P}(p_d) \sim \exp(-N\,\Delta F)$. This relation allows for tests of (30)–(32) in numerical simulations.

Finite dimensions

Let us now briefly comment about the relevance of our results for finite-dimensional spin glasses.

In addition to spin–spin correlations, an important quantity in finite dimensions is the correlation overlap function $\overline{\langle S_i S_j \rangle_1 \langle S_i S_j \rangle_2}$. In a chaotic situation this decays exponentially with a characteristic length $\xi_{1,2}$ for large $|i-j|$. This quantity was studied in [5, 6], where it was found that for $d > 8$

$$\xi_{0,h} \sim h^{-2/3} \qquad \text{and} \qquad \xi_{T_1,T_2} \sim |T_1 - T_2|^{-1}. \tag{33}$$

This behaviour was confirmed in numerical simulations by Ritort [14]. The sensitivity to small variations of an external parameter X is characterized by a 'chaos exponent' ζ, in $\xi_{X_1,X_2} \sim |X_1 - X_2|^{-1/\zeta}$, first considered in the framework of the scaling theory of Bray and Moore [15] and the droplet theory of Fisher and Huse [16].

These results (33) may be compared with ours via the relation found in [14]:

$$N[\delta p_d^2]_{\rm av} \sim \xi^4 \tag{34}$$

where $[\cdots]_{\rm av}$ denotes the average with respect to the distribution function of p_d, $\mathcal{P}(p_d) \sim \exp(-N\,\Delta F)$. Upon substituting our results for the free-energy excess ΔF one recovers the results (33) for the dimension-independent exponent ζ in the corresponding cases, in the case of two non-zero magnetic fields, for small $|h_1 - h_2| = \delta h$ our result is

$$\xi_{h_1,h_1+\delta h} \sim (h_1\,\delta h)^{-1/4}. \tag{35}$$

In lower dimensions it is possible to determine ξ_{T_1,T_2} [16–18] and ΔF [18] within the scaling theories. The differences compared with the mean-field case are that the relation between the two is different from (34), giving $\Delta F \sim \delta p_d^2 |T_1 - T_2|^{4/\zeta}$, the exponent ζ now depends on dimension and there are two regimes in temperature with two different behaviours of the two quantities mentioned [17] (one is the low-temperature phase, the other is the critical region). It could be interesting to see whether the latter happens in the mean-field case, too.

5. Conclusions

In this paper we have studied the correlations between states at different magnetic fields and temperatures in some spin-glass models. In the REM and GREM chaos is absent with temperature, while there is chaos with magnetic field. This is understood in simple terms based on the ultrametric construction of temperature-independent trees. As soon as a temperature dependence is assumed, considering correlated but not identical energy levels for different temperatures, chaos is present. This could provide a possible mechanism for the occurrence of chaos in microscopic models.

In the case of the SK model, we confirm the suggestions of Parisi [3] and Sompolinsky [4] that chaos is present both with respect to magnetic field and temperature changes. The question was previously investigated analytically by Kondor [5] and Kondor and Végsö [6], who reached conclusions similar to ours. We stress, however, the importance of our further analysis: the results of these latter authors were based on an ansatz in which the matrix P_{ab}

had all elements identical. Such a restriction would lead to the conclusion that chaos with respect to temperature is also present in models where this is manifestly not the case, as in the REM and GREM. It was then necessary to use a more general ansatz in replica space, allowing us to discern the chaotic from the non-chaotic behaviour. Near the critical temperature we find that if the magnetic fields or the temperatures in the two systems are different, an extensive amount of free energy has to be paid to impose an overlap greater than that corresponding to zero correlations. This implies that all the possible couples of states with different external parameters and free-energy density equal to that of the states dominating the partition function have minimal correlations. The scenario we find has implications for the physical picture of the low-temperature phase of the model. The hypothesis of successive bifurcations of the ultrametric tree as the temperature is lowered [12] is incompatible with our results.

In conclusion, let us comment on the fact that temperature-cycling experiments in spin-glass off-equilibrium relaxation [19] show strong correlations in the dynamics at different temperatures on finite time scales. If the physics of experimental spin glasses were similar to that of the SK model in this respect, one could expect these correlations eventually to decay to zero for large times. It would be very interesting in this context to test the finite-time behaviour of the SK model in simulated temperature-cycling experiments.

Appendix

In this appendix we show that no ultrametric solution of the kind discussed in section 2 exists for the SK model near T_c (4). We will show this by contradiction, assuming an ultrametric solution with $q_s(x)$ and $p(x)$ continuous in x. The discussion is done in the case of the complete model; the same argument could also be applied to the truncated model, with the same conclusions.

We discuss the case $h_1 = h_2 = 0$ and different temperatures; a similar (and simpler) proof leads to the conclusion that there is chaos with magnetic field. Let us write the variational equations for the complete model considering generic values of w, u, y, v:

$$2\tau_{rs}\mathbf{Q}_{\alpha\beta} + w(\mathbf{Q}^2)_{\alpha\beta} + \tfrac{2}{3}u\mathbf{Q}^3_{\alpha\beta} - y\sum_{\gamma}[\mathbf{Q}^2_{\alpha\gamma} + \mathbf{Q}^2_{\beta\gamma}]\mathbf{Q}_{\alpha\beta} + v(\mathbf{Q}^3)_{\alpha\beta} = 0. \tag{A1}$$

Plugging in the Parisi form of the matrices Q_s and P one get a set of coupled integral equations for the functions $q_s(x)$ and $p(x)$ that can be solved by repeated differentiation with respect to x.

For future reference we give the solution of the free case [20] at a temperature $\tau = (1 - T^2)/2$:

$$q_F(x) = \begin{cases} \dfrac{w}{2u}\dfrac{x}{\sqrt{1 + \frac{3v}{2u}x^2}} & x < \overline{x} \\ q(1) & x \geqslant \overline{x} \end{cases} \tag{A2}$$

where $q(x)$ is continuous in $\overline{x}$ and $q(1)$ is specified by the equation

$$2\tau + 2y\langle q^2\rangle - 2wq(1) + (3v + 2u)q(1)^2 = 0. \tag{A3}$$

In order to solve the problem we have to compute the Parisi functions associated with the various terms of (A1). In particular we need to compute the functions associated with

$$\mathbf{Q}^2 = \begin{pmatrix} Q_1^2 + P^2 & P(Q_1 + Q_2) \\ P(Q_1 + Q_2) & Q_2^2 + P^2 \end{pmatrix} \tag{A4}$$

and

$$\mathbf{Q}^3 = \begin{pmatrix} Q_1^3 + P^2(2Q_1 + Q_2) & P^3 + P(Q_1^2 + Q_2^2 + Q_1 Q_2) \\ P^3 + P(Q_1^2 + Q_2^2 + Q_1 Q_2) & Q_2^3 + P^2(Q_1 + 2Q_2) \end{pmatrix}. \tag{A5}$$

To do that, let us recall that the eigenvalues associated with a Parisi matrix $A \to (\tilde{a}_d, a(x))$ are

$$\lambda_0 = a_d - \langle a \rangle \qquad \text{with multiplicity 1} \tag{A6}$$

$$\lambda(x) = a_d - xa(x) - \int_x^1 \mathrm{d}y\, a(y) \qquad \text{with multiplicity } -n\frac{\mathrm{d}x}{x^2}. \tag{A7}$$

Observing that

$$\lambda'(x) = -xa'(x) \tag{A8}$$

one can invert the relation (A7) and get

$$a(x) = a(1) + \int_x^1 \mathrm{d}y\, \frac{\lambda'(y)}{y}. \tag{A9}$$

Let us denote by $\lambda_1(x), \lambda_2(x), \lambda_p(x)$ the eigenvalues associated with Q_1, Q_2, P, respectively. The eigenvalues associated with $\mathbf{Q}^2$ will be

$$Q_s^2 + P^2 \to \lambda_s^2(x) + \lambda_p^2(x) = {}^2\Lambda_s(x) \tag{A10}$$

$$P(Q_1 + Q_2) \to \lambda_p(x)[\lambda_1(x) + \lambda_2(x)] = {}^2\Lambda_p(x) \tag{A11}$$

($s = 1, 2$); the corresponding functions can be obtained from (A9), noting that as the magnetic field is zero $q_s(0) = p(0) = 0$,

$${}^2A_s(x) = 2\int_0^x \mathrm{d}y\, [\lambda_s(y)q_s'(y) + \lambda_p(y)p'(y)] \tag{A12}$$

$${}^2A_p(x) = 2\int_0^x \mathrm{d}y\, \{p'(y)[\lambda_1(y) + \lambda_2(y)] + [q_1'(y) + q_2'(y)]\lambda_p(y)\} \tag{A13}$$

having made use of (A8). The derivatives with respect to x of these functions are

$${}^2A_s'(x) = 2[\lambda_s(x)q_s'(x) + \lambda_p(x)p'(x)] \tag{A14}$$

$${}^2A_p'(x) = 2\{p'(x)[\lambda_1(x) + \lambda_2(x)] + [q_1'(x) + q_2'(x)]\lambda_p(x)\}. \tag{A15}$$

In a completely analogous way one finds the functions ${}^3A_s(x)$ and ${}^3A_p(x)$ and their derivatives:

$${}^3A_1'(x) = 3q_1'\lambda_1^2 + 2p'\lambda_p(2\lambda_1 + \lambda_2) + \lambda_p^2(2q_1' + q_2') \tag{A16}$$

$${}^3A_p'(x) = 3p'\lambda_p^2 + p'(\lambda_1^2 + \lambda_2^2 + \lambda_1\lambda_2) + \lambda_p(2\lambda_1 q_1' + 2\lambda_2 q_2' + \lambda_1 q_2' + \lambda_2 q_1'). \tag{A17}$$

The formula for ${}^3A_2'(x)$ is obtained from (A16) by interchanging the indices '1' and '2'. Observing that

$$\sum_\gamma [\mathbf{Q}_{\alpha\gamma}^2 + \mathbf{Q}_{\beta\gamma}^2] = \begin{cases} 2[p_d^2 - \langle p^2 \rangle - \langle q_s^2 \rangle] & r = s \\ 2[p_d^2 - \langle p^2 \rangle] - \langle q_1^2 \rangle - \langle q_2^2 \rangle & r \neq s \end{cases} \tag{A18}$$

and that the functions associated with $\mathbf{Q}_{\alpha\beta}^3$ are simply $q_s^3(x)$ and $p^3(x)$, one finds that *the derivatives with respect to* x of the saddle-point equations read

$$\begin{aligned} &[2\tau_1 - 2y(p_d^2 - \langle p^2 \rangle - \langle q_1^2 \rangle)]q_1' + 2w[p'\lambda_p + q_1'\lambda_1] \\ &\quad + v[3q_1'\lambda_1^2 + 2p'\lambda_p(2\lambda_1 + \lambda_2) + \lambda_p^2(2q_1' + q_2')] + 2uq_1^2 q_1' = 0 \end{aligned} \tag{A19}$$

a similar equation with $1 \leftrightarrow 2$, and

$$[2\tau_{12} - y(2(p_d^2 - \langle p^2\rangle) - \langle q_1^2\rangle - \langle q_2^2\rangle)]p' + w[p'(\lambda_1 + \lambda_2)) + (q_1' + q_2')\lambda_p] + v[3\lambda_p^2 p' + p'(\lambda_1^2 + \lambda_2^2 + \lambda_1\lambda_2) + \lambda_p(2\lambda_1 q_1' + 2\lambda_2 q_2' + \lambda_1 q_2' + \lambda_2 q_1')] + 2up^2 p' = 0. \quad \text{(A20)}$$

Let us now study the possibility of an ultrametric solution. Consider the 'small-x region' defined in (23), where $q_1(x) = q_2(x) = p(x) = f(x)$, and suppose $f'(x) \neq 0$. One can then differentiate (A19) repeatedly and find that

$$f(x) = q_F(2x). \quad \text{(A21)}$$

In the 'large-x region', where $p(x) = p_d$ observing that $\lambda_p(x) = 0$ there, one finds that the second equation is automatically satisfied, while the first two equations reduce to

$$q_s'[2\tau_s - 2y(p_d^2 - \langle p^2\rangle - \langle q_s^2\rangle) + 2w\lambda_s + 3v\lambda_s^2 + 2uq_s^2] = 0 \quad \text{(A22)}$$

that is, we get two uncoupled equations for q_1 and q_2 in this region. Again by repeated differentiation, we find that if $q_s' \neq 0$ then $q_s(x) = q_F(x)$. Using the assumption of continuity we find

$$q_s(x) = \begin{cases} q_F(2x) & x \leqslant x_0/2 \\ p_d & x_0/2 < x \leqslant x_0 \\ q_F(x) & x_0 < x \leqslant \overline{x}_s \\ q_s(1) & \overline{x}_s < x \leqslant 1 \end{cases} \qquad p(x) = \begin{cases} q_F(2x) & x \leqslant x_0/2 \\ p_d & x_0/2 < x \leqslant 1. \end{cases} \quad \text{(A23)}$$

The only free parameters at this level are the values $q_1(1)$ and $q_2(1)$. These can be fixed, e.g. by considering equation (A22) in $x = \overline{x}_s$ which gives

$$2\tau_s + 2y\left[\int_0^{\overline{x}_s} \mathrm{d}x\ q_F(x)^2 + (1 - \overline{x}_s)q_s(1)^2\right] - 2wq_s(1) + (3v + 2u)q_s(1)^2 = 0. \quad \text{(A24)}$$

This shows that $q_s(1)$ is equal to the value $q_F(1)$ corresponding to $\tau = \tau_s$. If now one inserts the resulting functions in equations (A19) one finds the contradiction

$$(p_d - \langle p\rangle)(\langle q_1\rangle - \langle q_2\rangle) = 0 \quad \text{(A25)}$$

showing the inconsistency of the hypothesis of an ultrametric solution except for the trivial one with $p_d = 0$.

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