Classification
Physics Abstracts
05.40 — 05.70 — 75.10 — 64.60

Short Communication
Self induced quenched disorder: a model for the glass transition

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Abstract. — We consider a simple spin system without disorder which exhibits a glassy regime. We show that this model can be well approximated by a system with quenched disorder which is studied with the standard methods developed in spin glasses. We propose that the glass transition is a point where quenched disorder is self induced; a scenario for which the 'cavity' method might be particularly well suited.

The problem of the glass state remains one of the major unsolved issues in condensed matter theory. Despite an enormous body of experimental and numerical data and quite detailed phenomenological theories [1-3], there is no fully satisfactory microscopic model for the glass state. The intense theoretical activity on spin-glasses and other disordered systems [4] stemmed in part because they retain 'half' of the complexity of glasses: given a disordered ('quenched') set of interactions, what is the thermodynamics of the 'spin' degrees of freedom, is there a low temperature spin glass phase? etc. The spin glass theory has indeed given birth to many seminal ideas which have been transferred to other glassy systems like proteins [5-7], rubber [8], or even glass itself [3]. One subtle aspect of glasses is that there is no clear *a priori* distinction between 'slow' degrees of freedom responsible for random interactions and 'fast' degrees of freedom equilibrating therein, although everything goes as if it were the case: quenched disorder is self-induced. A satisfactory glass theory requires a detailed mathematical description of this scenario (in fact implicit in the mode coupling theory [9]) and the identification of these 'slow' degrees of freedom.

In the following we shall show a possible way to get round this problem. We present a simple model, already studied in [10], [11], which contains no quenched disorder. At this stage, the

only justification for studying this model comes from numerical simulations : the system very clearly exhibits features of a glass transition - jump in the specific heat [11], slow dynamics and aging [12], etc. We propose an unusual analytical approach to this model which is to find a 'fiduciary' disordered model which is 'as close as possible' to the pure model, but for which all the ideas and methods developed for spin glasses (replicas, cavity method, statistics of the metastable states) are readily available. Our approach is the complete opposite of the usual one, which is to replace a 'dirty' system by an equivalent, 'pure' one. We show that the high temperature (replica symmetric) phase of our 'fiduciary' system reproduces exactly an approximation due to Golay [10], [11] for the original model, which, although unjustified, accounted reasonably well for Bernasconi's numerical data at high enough temperatures [11]. The entropy given by this approximation however becomes negative at low temperatures, signalling, for our fiduciary model, the breaking of replica symmetry. We find that the system undergoes a first order transition towards a low temperature (glass) phase which is rather similar to the low temperature phase of Derrida's random energy model [13], although the entropy remains non zero - reflecting the fact that small scale motions are not completely frozen. This random energy structure is in good agreement with the numerical findings of Bernasconi, who found that the energy landscape is 'golfcourse' like, with low energy states randomly distributed in phase space [11].

We shall first describe the specific model we considered and its fiduciary disordered version, and sketch the main steps of the calculations. We shall then turn to a more physical (and speculative) discussion on the relevance of the rather abstract model studied here for more realistic situations.

The model in question is defined by the following Hamiltonian:

$$\mathcal{H} = \frac{J_0^2}{2N} \sum_{k=1}^{N-1} \left[\sum_{i=1}^{N-k} S_i S_{i+k} \right]^2 \equiv \frac{J_0^2}{2N} \sum_{k=1}^{N-1} R_k^2 \tag{1}$$

where $S_{i=1,\dots,N}$ are Ising spins. The scaling of $\mathcal{H}$ with N has been chosen such that $\mathcal{H}$ is extensive. The spin configurations which minimize $\mathcal{H}$ are binary sequences with small autocorrelations, which are useful in communication engineering problems [11]. It is difficult to find them because of frustration effects.

As mentioned in the introduction, numerical studies show very clearly that the system enters a glassy phase at low temperatures, much as if quenched disorder were present. Furthermore, the non-trivial features of $\mathcal{H}$ come from the fact that the sum over k extends to infinity when $N \longrightarrow \infty$. In other words, it is the couplings between very far away spins which matter - suggesting that the one-dimensional nature of the problem might not be crucial. We thus propose to replace equation (1) by the following 'fiduciary' Hamiltonian:

$$\mathcal{H}_{\mathrm{d}} = \frac{1}{2N} \sum_{k=1}^{N-1} \left[\sum_{i=1}^{N} \sum_{j=1}^{N} J_{ij}^{(k)} S_i S_j \right]^2 \tag{2}$$

where $J_{ij}^{(k)}$ are random connectivity matrices, independent for different k's, with each element equal to J_0 with probability $(N-k)/N^2$ and zero otherwise. This choice insures that the average number of bonds in $\mathcal{H}$ and $\mathcal{H}_{\mathrm{d}}$ is precisely the same: note that the choice $J_{ij}^{(k)} \equiv J_0 \delta_{i+k,j}$ reproduces exactly equation (1). (J_0 is set to 1 in the sequel). $\mathcal{H}_{\mathrm{d}}$ can be considered as the mean field version of $\mathcal{H}$ where the geometry is lost. Interestingly, this mean field Hamiltonian allows one to use the replica formalism. The computation of the quenched free energy associated with H_{d}, using replicas, follows standard paths [4] which we cannot detail here. In the average of

Z^n, we first linearize the dependence on $J_{ij}^{(k)}$ through a Hubbard-Stratonovitch transformation. The auxiliary variables $q^{ab} = N^{-1} \sum_i S_i^a S_i^b$ are then introduced together with their Legendre parameters $\hat{q}^{ab}$: these allow us to decouple the various sites. Therefore, $\overline{Z^n}$ can be written in the following form, which allows a saddle point evaluation at large N:

$$\overline{Z^n} = \int \prod_{a<b} \mathrm{d}q_{ab}\mathrm{d}\hat{q}_{ab} \left(\mathrm{Tr}_{S_a} \exp \sum_{a<b} \hat{q}_{ab} S_a S_b \right)^N \exp\left[-N \sum_{a<b} q_{ab}\hat{q}_{ab} \right.$$

$$\left. + N \int_0^1 \mathrm{d}x \log\{ \int \prod_a \mathrm{d}\lambda_a e^{-\frac{\beta}{2}[(1+\beta(1-x))\sum_a \lambda_a^2 + \beta(1-x)\sum_{a\neq b} q_{ab}\lambda_a\lambda_b]} \} \right] \quad (3)$$

from which the free-energy F_d at temperature $1/\beta$ is obtained, through $F_\mathrm{d} \equiv (-1/(N\beta)) \times \lim_{n\to 0} \partial \overline{Z^n}/\partial n$.

Let us first describe the replica symmetric saddle point of (3), with $q_{a\neq b} \equiv q$ and $\hat{q}_{a\neq b} \equiv \hat{q}$. We find that $q_\mathrm{saddle} = \hat{q}_\mathrm{saddle} = 0$, leading to $F_\mathrm{d}^\mathrm{RS} = -\beta^{-1} \int_0^1 \mathrm{d}x \log[1+\beta(1-x)]$. Interestingly, this free energy coincides *exactly* with the one obtained by Golay [10] for the original model equation (1), under the (unjustified) assumption that $R_k \equiv \sum_{i=1}^{N-k} S_i S_{i+k}$ are Gaussian independent variables. As shown numerically by Bernasconi, F_d^RS gives a rather good description of the 'high' temperature region. This solution however suffers from the usual entropy disease, which becomes negative below a certain temperature $T^* = 0.047564...$ and goes to $-\infty$ for $T = 0$. However, there is no sign of local instability, suggesting that the transition to a replica symmetry broken phase must be first-order (from the point of view of the order parameter function: as we shall see, the transition is second order from the thermodynamical point of view). As shown in detail in [14], the existence of a phase transition is ensured by the fact that $\overline{Z^2} \simeq \overline{Z}^2$ at high enough T. The one step replica symmetry broken solution allows us to introduce, as usual, a minimal and a maximal overlap q_0, q_1, as well as the position of the 'breakpoint' m, connected with the density of low-lying states (and in turn with the dynamical properties [15], [16]). We find that $q_0 \equiv 0$ and $m(T) \simeq T/T_\mathrm{g}$ with $T_\mathrm{g} = 0.047662 > T^*$, while $y(T) \equiv \beta(1-q_1^2)$ behaves as shown in figure 1. Figures 2a, 2b show the free energy and the entropy in the low temperature phase $T < T_\mathrm{g}$. Note that the entropy is everywhere positive but rather small ($\simeq 10^{-5}$ per spin), goes to zero linearly with T (as in real glasses), and matches that of F_d^RS at $T = T_\mathrm{g}$. T_g thus appears as a freezing temperature at which q_1 discontinuously jumps from zero to a value rather close to 1 (Note the scale in Fig. 1). The specific heat also jumps at T_g. The picture of the glass phase is rather similar to that of the random energy model, for which [13], [17] $q_0 \equiv 0$, $m(T) \equiv T/T_\mathrm{g}$ but also $q_1 \equiv 1$ corresponding to the fact that the entropy of the frozen phase is strictly zero - at variance with our model for which a residual entropy remains. Our prediction for the ground state energy is $E_\mathrm{GS} = 0.02028455....$ Bernasconi noted that the numerical ground state energy was much higher than this value as soon as $N \geq 50$, which might simply reflect the fact that if the energy landscape is that of the random energy model, it is extremely difficult to find the ground state. The apparent freezing temperature found in [11, 18] is also a factor $\simeq 2$ larger than our T_g (note the difference in normalization between our work and Bernasconi's). This discrepancy might be due either to the fact that our fiduciary model is not appropriate and fails to reproduce the correct T_g, or to the fact that the simulated annealing of [11, 18] gets trapped into deep metastable states as soon as T reaches $T_\mathrm{dyn} > T_\mathrm{g}$. This is a likely scenario in view of the very glassy nature of the system. A more systematic numerical study is however needed to settle this point.

It could be that a more complicated replica symmetry breaking scheme is needed. We however think that the numerical differences with our results are likely to be extremely small;
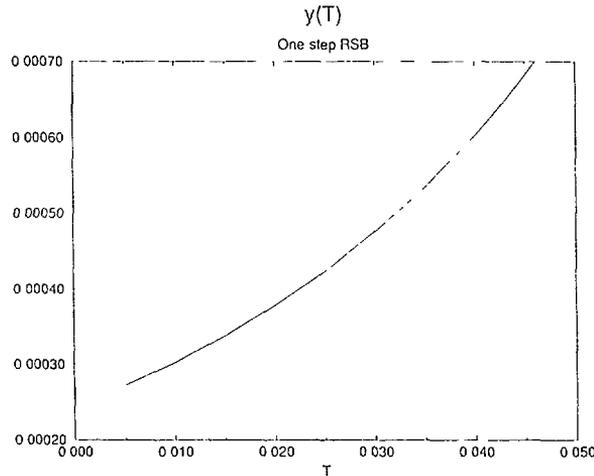
Fig. 1. — Plot of the quantity $y(T) \equiv (1 - q_1^2(T))/T$ in the low temperature phase. Note the scale, which indicates that the deviations of q_1 from 1 are very small.

it is furthermore irrelevant to the point addressed in this letter. We shall now discuss the above results from a more physical point of view. Although quite remote from reality, the model we considered illustrates the fact that a pure model can undergo a glass transition which can be described using the tools of disordered systems since its mean field formulation naturally introduces random variables. Breaking of replica symmetry indicates, as usual, the existence of many (metastable) states, and its physical meaning is best understood in the 'cavity' approach [4], which is essentially based on a certain (hierarchical) construction of the equilibrium states and the local field distribution. In disordered systems, this method is *in fine* equivalent to the replica calculation. In the pure model at hand, however, the cavity method in fact allows us to recover all the above results without introducing a fiduciary random Hamiltonian, but rather through adequate hypotheses on the statistics of the S_i and the R_k [19]. Within a one pure state picture ('replica symmetric'), the only viable assumption is that $< S_i >\equiv 0$, which immediately leads back to Golay's approximation. The existence of many 'states' α with weight P_α however allows us to go beyond this result, since it is possible to have $\sum_\alpha P_\alpha < S_i >_\alpha \equiv 0$ but $\sum_\alpha P_\alpha < S_i >_\alpha^2 = q_1 \neq 0$. In other words, if the spins are frozen in a given state, the field acting on the extra ('cavity') spin will be much like a quenched random variable. A simplistic way to express this idea might be the following: one can rewrite equaion (1) as

$$\mathcal{H} = \sum_{i,j} \frac{J_{ij}}{2\sqrt{N}} S_i S_j \tag{5}$$

with $J_{ij} \equiv \dfrac{J_0}{\sqrt{N}} \sum_k S_{i+k} S_{j+k}$, i.e. as a spin-glass SK Hamiltonian but for which the couplings *are themselves determined by the spins.* However, if the dynamics of the system is slow (which it is in the 'spin-glass' phase) then the couplings can be self-consistently thought of as quenched random variables. This suggests that the scenario described here is far more general [9] and that a genuine short range model of glass could be a pure four spin interation Hamiltonian of the form $\mathcal{H}_4 = -J \sum_{<ijkl>} S_i S_j S_k S_l$, where $< ijkl >$ denotes, for example, nearest neighbour tetrahedra on a cubic lattice. $\mathcal{H}_4$ obviously possesses a 'crystalline' ground state $S_i \equiv 1$.

Free energy

One step RSB

a)

Entropy in the frozen phase

(Note the scale)

b)
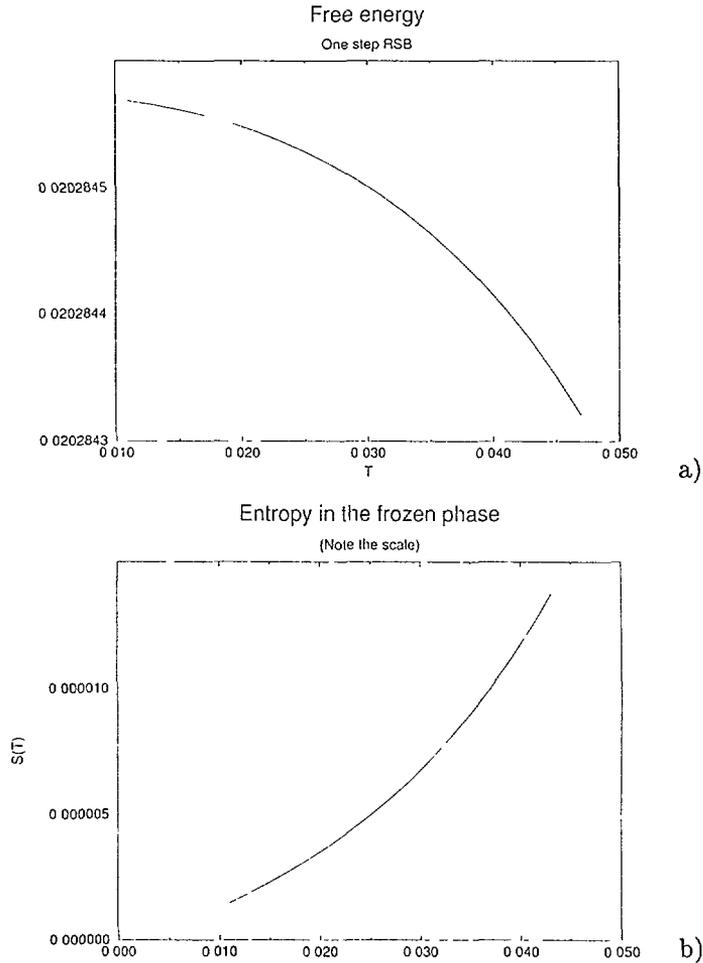
Fig. 2. — Plot of the free-energy (2a) and entropy (2b) in the glass phase. Note that $S(T)$ is positive but rather small. We found that $S(T) = AT$ (for small T) with $A \simeq 5 \times 10^{-5}$

If, however, the system is quenched from high temperature, the $\{S_i\}$ are initially random and generate random effective couplings J_{ij}, which, if the temperature is sufficiently small, will very slowly evolve and lead to a 'self consistent' spin-glass. Numerical simulations [20] show that this is indeed the case: glassy dynamics and aging very similar to that observed in experimental spin glasses are clearly observed. Of course, if the interaction is of finite range, this quenched effective disorder will progressively anneal out (possibly on astronomical time scales), allowing the system to find its crystalline state - as indeed in real glasses. Only if the interaction is of infinite range, like in the models considered above, or if some topological constraints forbid the annealing of disorder [21] will this glass transition acquire a precise thermodynamical meaning. It is clear, however, that the range of interactions need not be very large for this limit to be relevant to experimental time scales [22]: in this work, we have primarily focused on static calculations, leaving the investigation of the dynamics (along the lines of [23], [24]) for future work. A dynamical approach is clearly needed in order to identify which internal degrees of

freedom get quenched and to make a link with the mode coupling theory [9]. The success of the present approach might indicate that the precise decomposition of which degrees of freedom become quenched or annealed is maybe not so crucial.

Acknowledgments.

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