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The fully frustrated hypercubic model is glassy and aging at large D

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Abstract. We discuss the behaviour of the fully frustrated hypercubic cell in the infinite-dimensional mean-field limit. In the Ising case the system undergoes a glass transition, well described by the random orthogonal model. Under the glass temperature aging effects show clearly. In the XY case there is no sign of a phase transition, and the system is always a paramagnet.

Recently there has been renewed interest in the study of deterministic models (without quenched disorder) with a complex low-temperature behaviour [1–3] (for more details about the dynamics see [4,5]; for additional developments see [6,7]). In our first paper [1] we have discussed the low autocorrelation model, and solved it by using replica theory. In the second paper of the series [2] we have introduced another class of models that share the same crucial features, which are in some sense more generic than the low autocorrelation sequences. Let us briefly describe them. They are, as we have already said, deterministic models, which do not contain frozen disorder. Their Hamiltonian is based on a long-range interaction

$$H \equiv -\sum_{x,y} J_{x,y}\sigma_x\sigma_y \tag{1}$$

where the indices x and y run from 1 to the number of sites N. The couplings $J_{x,y}$ are not random variables, but are defined as (*sine model*)

$$J_{x,y} = \frac{1}{\sqrt{2N+1}}\sin\left(\frac{2\pi xy}{2N+1}\right). \tag{2}$$

We notice [1,2] at first that the high-temperature expansion of this class of models can be computed in a straightforward way after noticing that the couplings $J_{x,y}$ form an orthogonal matrix. By proceeding on the same lines, the model defined by the Hamiltonian (1) can be solved completely. One substitutes the orthogonal $J_{x,y}$ matrix with a distribution of generic orthogonal random matrices, integrates over them (we call this model the random orthogonal model, ROM), and solves the model by using replica theory. The solutions of the random model (based on generic orthogonal coupling matrices) and the deterministic model coincide, both in the high-T phase and in the spin-glass low-T phase (but for special properties that the deterministic model can have for special N values at low T).

The static and dynamical behaviour of these systems can now be understood from the point of view of the usual analysis of disordered systems. They show two very distinct transitions. The first one, at T_{RSB}, corresponds to the usual static transition. Here replica symmetry breaks. At $T = T_{\mathrm{RSB}}$ the entropy is very small†.

The other transition appears in the solution of the dynamical behaviour. We call it the glass transition temperature T_{G}. Below this temperature strong non-equilibrium effects start to appear. In [1] we have shown that this transition exists even in the deterministic models we have described previously.

In this paper we will show that the hypercubic fully frustrated Ising lattice model in the limit of an infinite number of dimensions undergoes a glass transition of the same kind as the one we found in the low autocorrelation and the sine model. We will show that such a glass transition is well described by the ROM. We will show that the model undergoes aging. The glass transition only exists for Ising-like variables. We will show that in the XY case of continuous, compact variables there is no phase transition. Here the system is always paramagnetic, and the $T = 0$ ground state is reached smoothly when cooling from high T.

The Hamiltonian of the fully frustrated lattice model is

$$H \equiv -\frac{1}{\sqrt{D}} \sum_{(x,y)} J_{x,y} s_x s_y \qquad |s_x| = 1 \tag{3}$$

where the sites x lie on a hypercubic cell in D dimensions (i.e. the x can take the values $[0, 1]^D$), and the sum runs over all nearest-neighbour couples. The $J_{x,y}$ couplings take the values ± 1, and are such that all plaquettes are frustrated (i.e. the product of the J's along the bonds of each plaquette is -1). The s_x variables live on the n-dimensional sphere, where n is the number of components of the spin vectors. $n = 1$ for the Ising case and $n = 2$ in the XY case.

The condition of being fully frustrated can be implemented in an infinite number of ways. We have used two of them which are gauge equivalent (one can go from one to the other by a gauge transformation on the J and the spins). We know about the first one from lattice gauge theories as a tool for discretizing lattice fermions [9]. μ and ν run over the lattice directions, from 1 to D, and one sets

$$J_{x,y} \equiv J(x_\mu, x_\mu + e_\nu) = (-1)^{\sum_{\mu<\nu} x_\mu} . \tag{4}$$

Here x_μ labels the D components of the coordinates of the site x, and e_ν is the unit vector in the direction ν, which connects the site x to the site y. The J in the direction 1 have the value $+1$. The $J_{x,y}$ form an orthogonal matrix, strengthening our expectation that the dynamical behaviour of this model will be described by the ROM.

We have also used (luckily enough with identical results) the construction suggested in [10, 11], which can be defined by induction. Let us take in $D = 1$ all couplings equal to 1. Now we define how to construct a fully frustrated $(D + 1)$-dimensional simplex when given a D-dimensional one. One just has to duplicate the D-dimensional simplex, multiply all coupling of the second copy times -1 (i.e. flipping all links), and join the corresponding sites of the two simplicia with $+1$ couplings. It is easy to see that this procedure generates a fully frustrated lattice in $D + 1$ dimensions.

We have also used a hypercubic lattice in D dimensions. On our lattice (a single cube) there are 2^D spins, and each spin is connected to D first neighbouring sites.

† In the context of structural glasses T_{RSB} corresponds to the Kauzmann temperature [8].

Former work on the subject is contained in [10–13]. Let us first focus on the Ising case ($n = 1$). It is easy to see [10, 11] that a lower bound for ground-state energy E_0 of the model is (given the normalization of (3))

$$E_0 \geqslant -\tfrac{1}{2}\,. \tag{5}$$

Also one can see that this bound is independent from the number of spin components n.

For Ising spins the bound (5) can be improved [10] in the cases where the dimension is not a square integer. The constraint that all spins are integer implies that non-trivial Diophantine equalities have to been satisfied from admissible spin configurations. The authors of [10] succeed in exhibiting a class of spin configurations that saturates the improved bound up to $D = 7$. For $D \geqslant 8$ they cannot be sure if configurations that satisfy their bound exist.

We have used a cooling procedure and a Monte Carlo annealing scheme (simulating from high temperatures T a thermal cycle down to $T = 0$) to gather information about the ground-state structure. Let us note at first that the simple cooling procedure is not efficient, and that the Monte Carlo annealing is crucial to get reasonable results.

For D going from 3 to 7 we find the same ground state exhibited in [10]. In $D = 6$ we confirm that only configurations corresponding to the first solution of table 1 of [10] are realizable, and that the other solution of the Diophantine equation seems not to correspond to any spin configuration. In $D = 8$ we have been able to exhibit the ground state corresponding to the improved energy lower bound.

In $D = 9$, the most accessible perfect square D value after the easy case of 4, we have not been able to access a ground state saturating the $-\frac{1}{2}$ bound, but we have reached a value very close to that, $-0.494\,792$. To give the scale we notice that on a scale where the minimal energy jump is 1 the ground-state energy is -384. On this scale we have reached a value† of -380, where the improved lower bound at $D = 8$ gives -361, while at $D = 10$ it gives -364. We give these numbers to make it clear that we have found the case $D = 9 = 3 \times 3$ admits an especially deep ground-state energy valley. For $D \geqslant 10$ we do not converge to the ground state. It is also interesting to notice that in the case $D = 16$ we do not succeed in going especially low in our search of the ground-state energy (the result of our search for $D = 16$ is not far better than for $D = 15$). The picture one is uncovering here is very much similar to that of the deterministic models of [1, 2], the main difference being that here we have corrections of order $1/D$ (which makes the fully frustrated model closer to the low autocorrelation model than to the sine model). There are special values of the number of elementary bits for which the system ground state is very low. The free-energy landscape is very much golf-course-like. Deep valleys are very steep, and impossible to find in the limit of large volume. The thermodynamical behaviour of the system is not influenced from these special minima.

After discussing the $T = 0$ properties of the system, we investigated its finite-T thermodynamical properties. The methods we introduced in [1, 2] (where we address the reader interested in the details of the computation) allow us to solve the model easily, by using the ROM analogy. One starts by substituting the interaction matrix $J_{x,y}$ (which, we noticed, happens to be an orthogonal matrix) by a generic random orthogonal matrix. The new disordered model is defined by means of the group-invariant integration over orthogonal matrices. Replica theory allows us to get a solution for this model, and replica-symmetry breaking allows us to deal with the model even when deep in the broken phase. In the high-T region, where the physical solution is replica symmetric, one finds that the free-energy

† We are four elementary units away from the improved bound value, but very probably the spin configuration is completely different from the correct ground state.

density f and the energy density e are given by

$$f = -\frac{1}{2\beta}G(\beta) - \frac{1}{\beta}\log(2) \qquad e = -\frac{G'(\beta)}{2} = -\frac{\sqrt{1+4\beta^2}-1}{4\beta} \tag{6}$$

where the function $G(z)$ is given by

$$G(z) = -\tfrac{1}{2}\log\left(\frac{\sqrt{1+4z^2}+1}{2}\right) + \tfrac{1}{2}\sqrt{1+4z^2} - \tfrac{1}{2}\,. \tag{7}$$

The high-T result coincides with the one derived in [11] by means of diagrammatic expansion, and re-obtained in a different framework in [13]. The entropy of the high-T replica-symmetric solution becomes negative below the replica-symmetry-breaking point at temperature $T_{\mathrm{RSB}} \simeq 0.0625$. Since we are dealing with spin variables that can only take discrete values this necessarily means that there has to be a phase transition close to T_{RSB}. Following the strategy we discussed in [1,2] we can solve the replica equations by implementing the marginality condition. The method seems to work very well to find [1,2] the dynamical glassy temperature, T_{G}. At T_{G} the system enters a glassy phase. Applying the marginality condition we obtain a glass transition temperature $T_{\mathrm{G}} \simeq 0.14$. Below this temperature we expect the dynamics to become very slow. Energy relaxes to its equilibrium value on exponentially large time-scales. In the glassy phase we expect the energy to stay close to its value at T_{G}, $E_{\mathrm{G}} \simeq -0.47$.

We have run Monte Carlo simulations of the fully frustrated model for different values of the dimensionality, up to $D = 17$. We started our runs from a random initial configuration at $T = 0.5$ and slowly decreased the temperature. We show in figure 1 the energy from our Monte Carlo runs as a function of the temperature for $D = 16$, together with a numerical simulation of the ROM model. The theoretical value in the cold phase is obtained by using the marginality condition (see [2] for details). The results strongly fluctuate depending on the space dimensionality (i.e. in our case depending on the volume). It is important to notice that, compared to the models we have discussed before in [1,2], the fully frustrated Ising hypercube has very strong finite-D effects. That is connected to the fact that the energy at the glassy transition, $E_{\mathrm{G}} \simeq -0.47$, is close to the energy of the ground state for low values of D. Only in the regime where $E_0(D) \ll E_{\mathrm{G}}$ do we expect to be able to get a clear picture

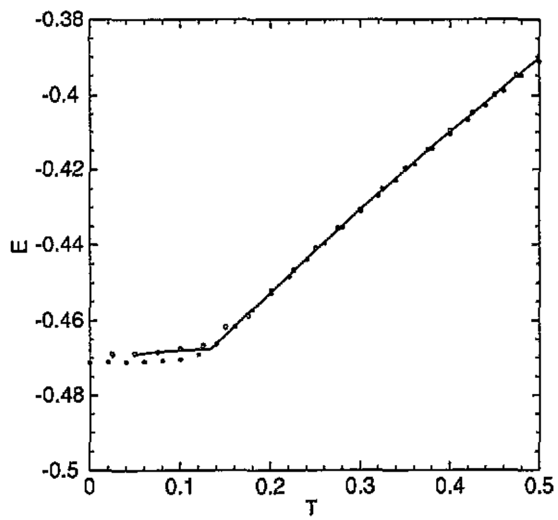

Figure 1. Energy of the Ising fully frustrated hypercubic cell for $D = 16$ as a function of the temperature (full circles). With open circles we report the results of numerical simulations of the ROM ($N = 186$). The full curve is the theoretical prediction for the ROM (in the cold phase the result is computed by assuming the marginality condition).

of the glass transition. This is what starts to happen for the higher values of D we have been able to study.

We discuss next in more detail the dynamical behaviour of the system. We expect that above the glass temperature T_G the system behaves as a paramagnet and time correlation functions decay very quickly to zero. Below T_G aging effects appear, and the decay rate of the time correlations depends on the history of the system. This is a common scenario in disordered systems [14, 15]. We have measured the spin–spin correlation function

$$C(t_w, t_w + t) = \frac{1}{N} \sum_{i=1}^{N} s_i(t_w) s_i(t_w + t) \qquad (8)$$

i.e. the correlation of the spins after a waiting time t_w with those after successive t steps. We have observed that the shape of the correlation function fluctuates when changing the dimension, even for very large sizes. This reflects how strong the finite-dimensional corrections are in the metastable glassy phase. In figure 2 we show the aging curves at

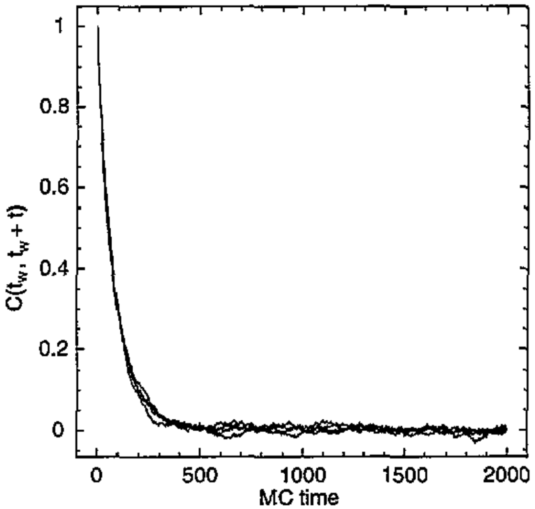

Figure 2. The correlation function C for for $T = 0.20$ and $D = 15$. $t_w = 25$, 100, 400 and 1600. Here there is no aging.

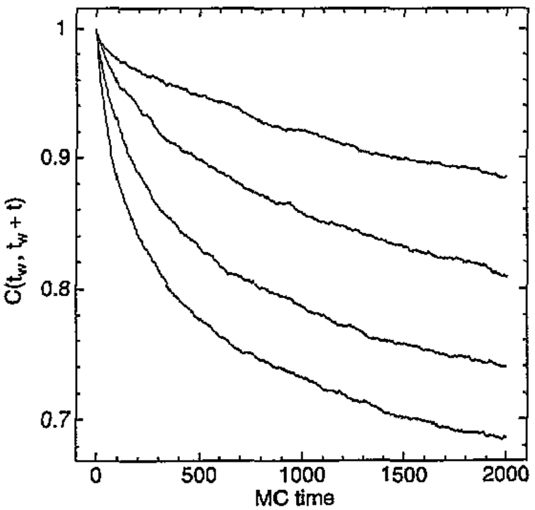

Figure 3. As in figure 2, but $T = 0.10$. Here aging is very clear.

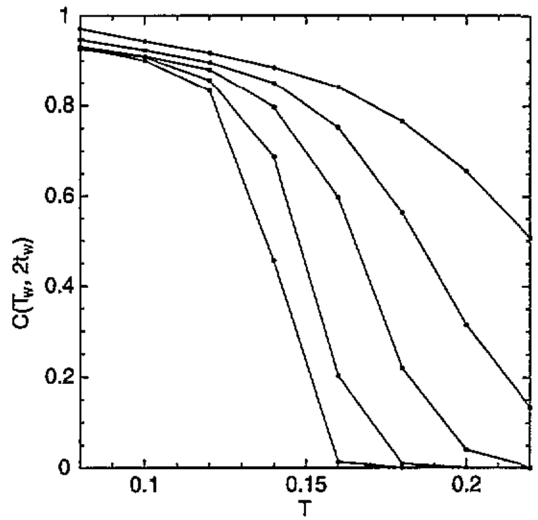

Figure 4. $C(t_w, 2t_w)$ as a function of the temperature for different values of t_w = 30, 100, 300, 1000, 3000 and $D = 17$. Lower curves are for higher values of t_w.

$T = 0.20$ for different waiting times in the case $D = 15$. Here we are in the paramagnetic phase, and there is no aging. In figure 3 we analyse the same correlation functions in the broken phase, at $T = 0.10$. Now the aging is very clear.

To make explicit the discontinuous nature of the glass transition we have measured the correlation function $C(t_w, 2t_w) = q(T)$ at different temperatures. This technique has been applied recently in the case of low autocorrelation models [5] and it seems a very good tool to pinpoint the location of the glass transition. The results are shown in figure 4. In the limit of large values of t_w we expect $q(T)$ to be zero above T_G. On the contrary q experiences a discontinuous jump just below T_G.

The body of the results we have discussed for the fully frustrated Ising model supports the standard scenario derived from the study of the ROM. Now we present our results obtained for the XY model, where the spin variables are complex numbers constrained to be of modulo 1 (and the J variables are the same as before). Here the system seems always to be able to find its exact ground state (with $E_0 = -\frac{1}{2}$), and we have not found any evidence of the existence of a phase transition. The whole phase diagram in T is well described by the high-temperature expression of (6) (after normalizing the temperature by the number n of spin components, $n = 2$ in the XY case). We show our results in figure 5, where we plot the internal energy of the model together with the high-temperature result. In the whole T-region finite-dimensional corrections are negligible, in agreement with the fact that the phase-space structure is very simple. We expect similar conclusions to be valid in case of Heisenberg or spherical spins. As far as we can understand from these results, frustration without quenched disorder needs to be helped from the discrete nature of the spin variables in order to create traps dangerous enough to enforce a complex behaviour.

We have shown that the Ising fully frustrated hypercubic cell in the high-D mean-field limit displays a low-T glassy behaviour. This model has a glass transition of a discontinuous type, well described by the solution of the random orthogonal model. We have noticed that the dynamical low-temperature behaviour is very sensitive to the finite-D corrections. We have also investigated the XY model. Here there is no sign of a phase transition and the system is always paramagnetic. It would be very interesting to understand if such a glassy behaviour is shared by usual short-ranged frustrated non-disordered models.

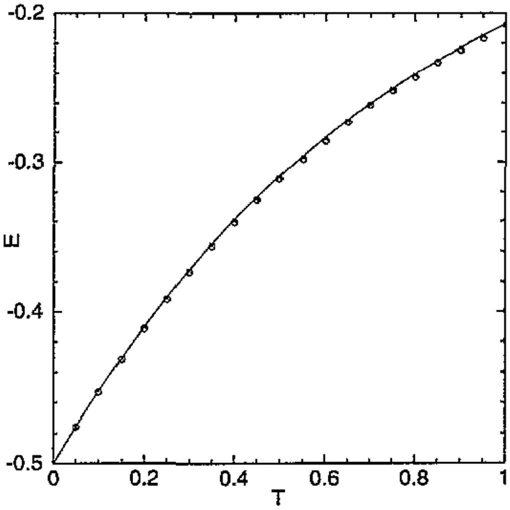

Figure 5. Energy of the fully frustrated hypercubic cell (XY model) for $D = 8$ (open circles) and $D = 15$ ($\times$) as a function of the temperature T. The full curve is the high-temperature prediction. There is no sign of the presence of a phase transition.

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