The Fully Frustrated Hypercubic Model is Glassy and Aging at Large D

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Abstract

We discuss the behavior 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.

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Recently there has been a renewed interest in the study of deterministic models (without quenched disorder) with a complex low temperature behavior [1, 2, 3] (for more details about the dynamics see [4, 5], for additional developments see [6, 7]). In our first paper, ref. [1], we have discussed the low autocorrelation model, and we have solved it by using replica theory. In the second paper of the series, ref. [2], we have introduced an other class of models that share the same crucial features, which are in same 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 they are defined as (*sine model*)

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

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 of 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 behavior 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 $T = T_{RSB}$ the entropy is very small[1].

The other transition appears in the solution of the dynamical behavior. 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 before.

In this note 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 of the one we have 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 exists only for Ising-like variables. We will show that in the XY case of continuous, compact variables there is no phase transition. Here

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

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

$$H \equiv -\frac{1}{\sqrt{D}} \sum_{(x,y)} J_{x,y}\ \mathbf{s}_x \mathbf{s}_y\ , \quad |\mathbf{s}_x| = 1\ , \tag{3}$$

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 neighbor 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 $\mathbf{s}_x$ 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 infinity 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 to discretize 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 behavior of this model will be described by the ROM.

We have also used (luckily enough with identical results) the construction suggested in ref. [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 neighboring sites.

Former work on the subject is contained in ref. [10, 11, 12, 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 eq. (3))

$$E_0 \geq -\frac{1}{2}\ . \tag{5}$$

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 to exhibit a class of spin configurations that saturates the improved bound up to $D = 7$. For $D \geq 8$ 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 ref. [10]. In $D = 6$ we confirm that only configurations corresponding to the first solution of table I 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, $-.494792$. 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[2] 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 clear we have found that the case $D = 9 = 3 \cdot 3$ admits a specially deep ground state energy valley. For $D \geq 10$ we do not converge to the ground state. It is also interesting to notice that in the case $D = 16$ we do not succeed to go 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 the one of the deterministic models of [1, 2], the main difference being that here we have corrections of order $\frac{1}{D}$ (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 bit 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 behavior of the system is not influenced from these special minima.

After discussing the $T = 0$ properties of the system we have been investigating its finite T thermodynamical properties. The methods we have introduced in [1, 2] (where we address the reader interested in the details of the computation) allow 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 to get a solution for this model, and replica symmetry breaking allows to deal with the model even deep in the broken phase. In the high T region, where the physical solution is replica symmetric, one finds that the free energy density f and the energy density e are given by

[2] We are 4 elementary units far from the improved bound value, but very probably the spin configuration is completely different from the correct ground state.

$$
\begin{aligned}
f &= -\frac{1}{2\beta}G(\beta) - \frac{1}{\beta}\log(2) \ , \\
e &= -\frac{G'(\beta)}{2} = -\frac{\sqrt{1+4\beta^2}-1}{4\beta} \ ,
\end{aligned}
\tag{6}
$$

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

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

The high T result coincides with the one derived in ref. [11] by means of diagrammatic expansion, and reobtained 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 $T_{RSB} \simeq 0.0625$. Since we are dealing with spin variables that can only take discrete values that 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 $T_G \simeq 0.14$. 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, $E_G \simeq -0.47$.

We have run Monte Carlo simulations of the fully frustrated model for different values of the dimensionality, up to $D = 17$. We have been starting our runs from a random initial configuration at $T = 0.5$ and we have 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, $E_G \simeq -0.47$, is close to the energy of the ground state for low values of D. Only in the regime where $E_0(D) \ll E_G$ we expect to be able to get a clear picture 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 behavior of the system. We expect that above the glass temperature T_G the system behaves as a paramagnet and time correlation functions decay very fast 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

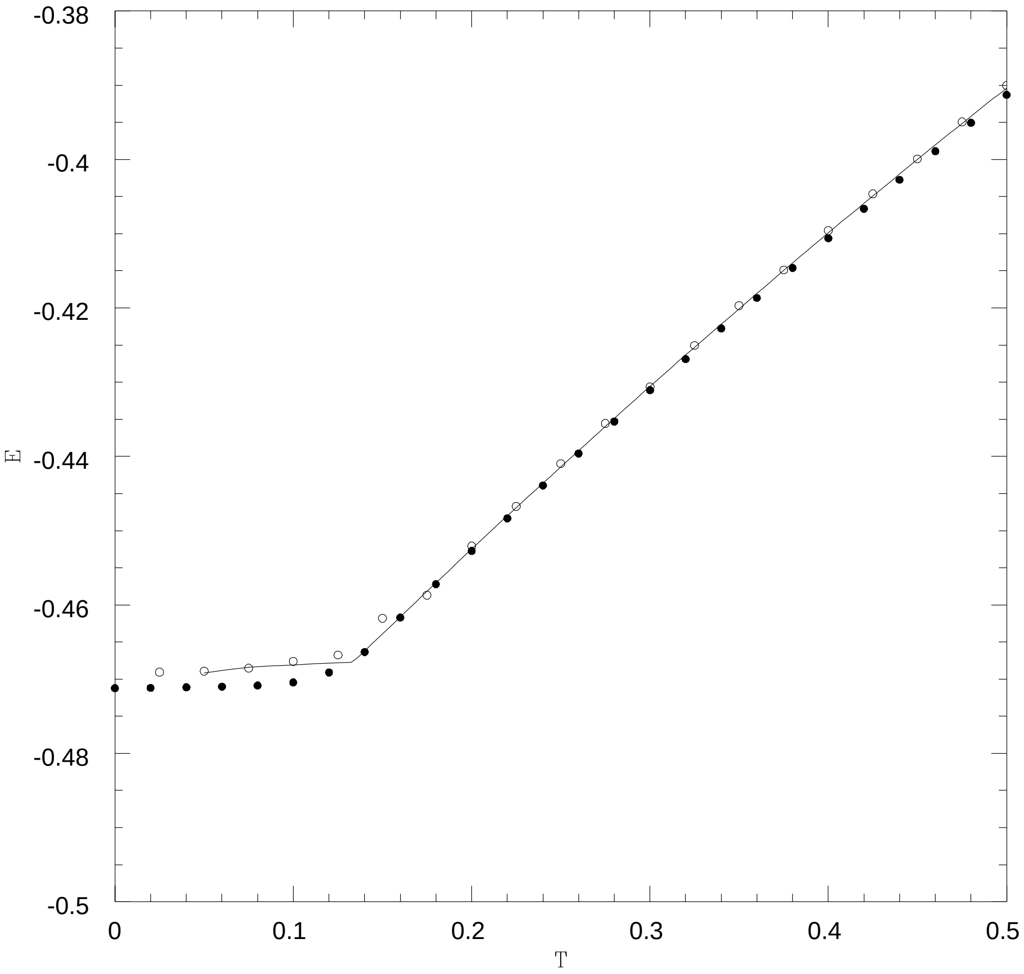

Figure 1: Energy of the Ising fully frustrated hypercubic cell for $D = 16$ as a function of the temperature (filled dots). With empty dots we report the results of numerical simulations of the ROM (N=186). The continuous line is the theoretical prediction for the ROM (in the cold phase the result is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

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

i.e. the correlation of the spins after a waiting time t_w with the ones after the 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 are the finite dimensional corrections also in the metastable glassy phase. In figure (2) we show the aging curves at $T = 0.20$ for different waiting times in the case $D = 15$. Here we are in the paramagnetic phase, and there is no aging. In next figure (3) we analyze the same correlation functions in the broken phase, at $T = .10$. 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 eq.(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 behavior.

We have shown that the Ising fully-frustrated hypercubic cell in the high D mean-field limit displays a low T glassy behavior. 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 behavior 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 behavior is shared by usual short-ranged frustrated non-disordered models.

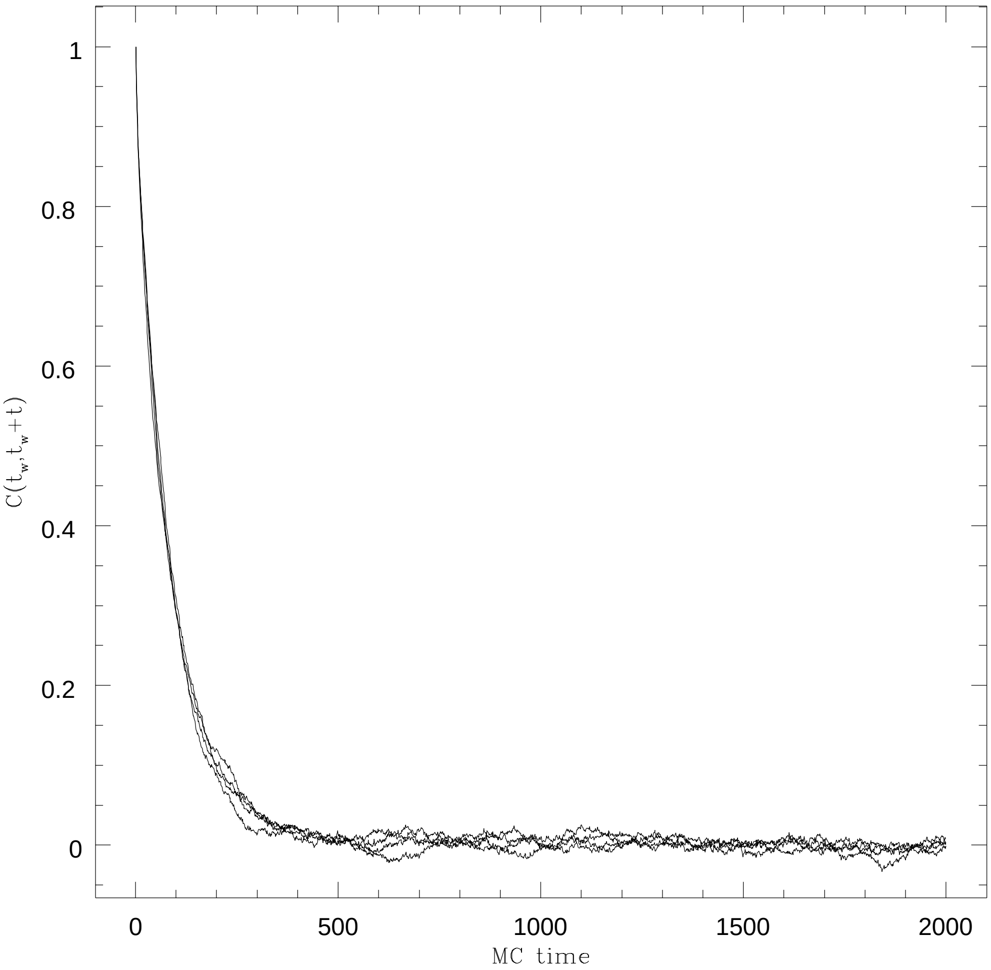

Figure 2: The correlation function C for for $T = 0.20$ and $D = 15$. $t_w = 25$, 100, 400 and 1600. Here there is no aging.

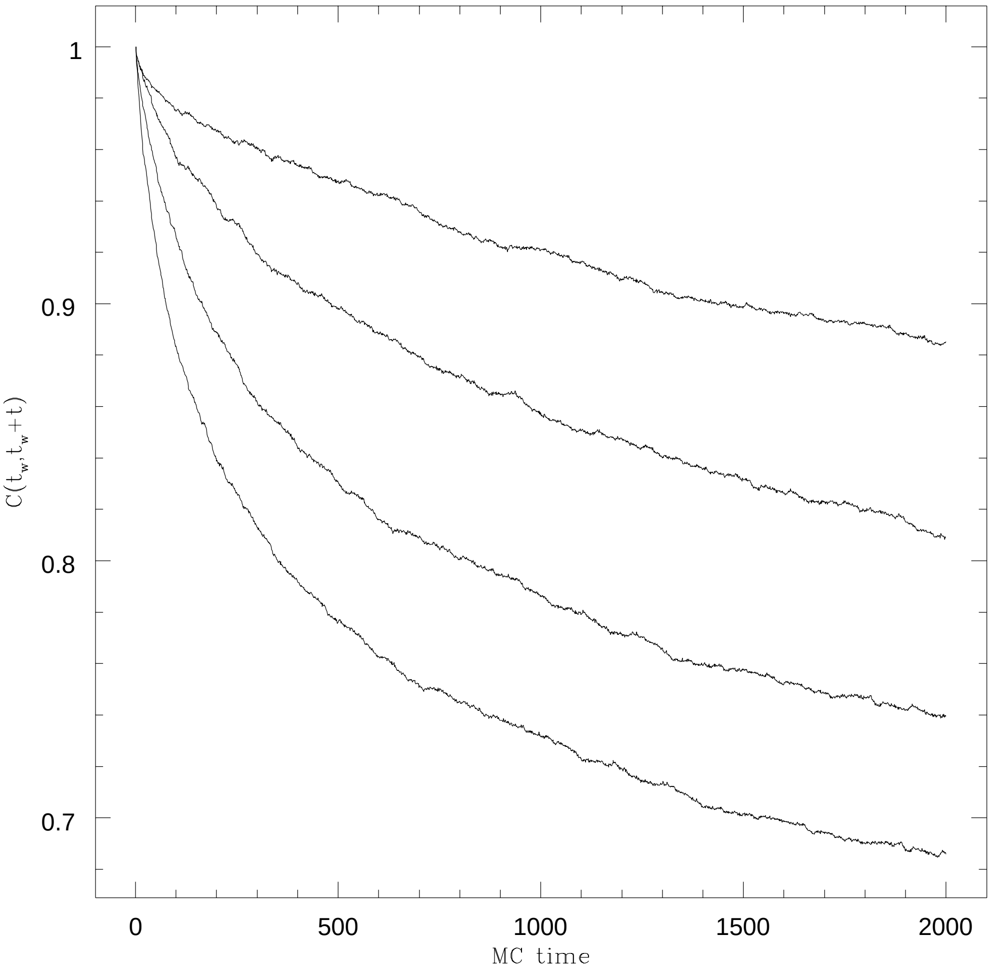

Figure 3: As in figure (2), but $T = 0.10$. Here aging is very clear.

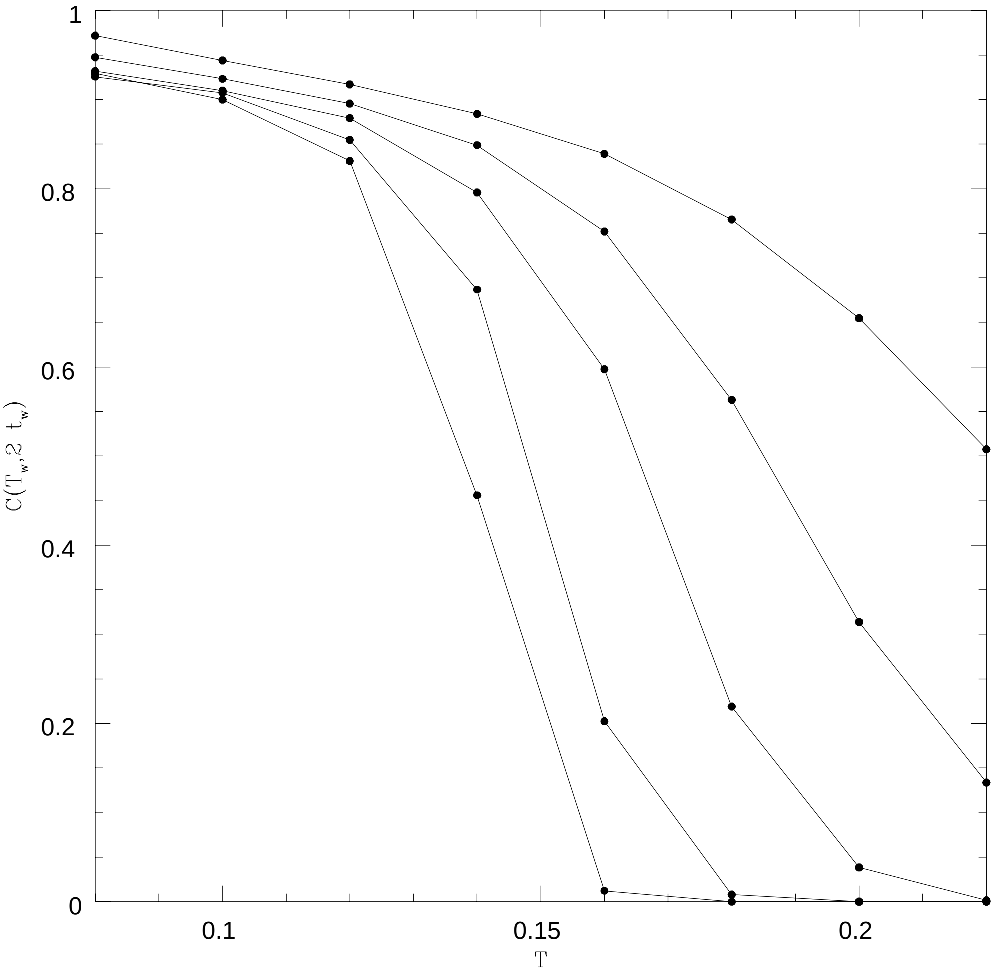

Figure 4: $C(t_w, 2t_w)$ as a function of the temperature for different values of $t_w = 30, 100, 300, 1000, 3000$ and $D = 17$. Lower curves are for higher values of t_w

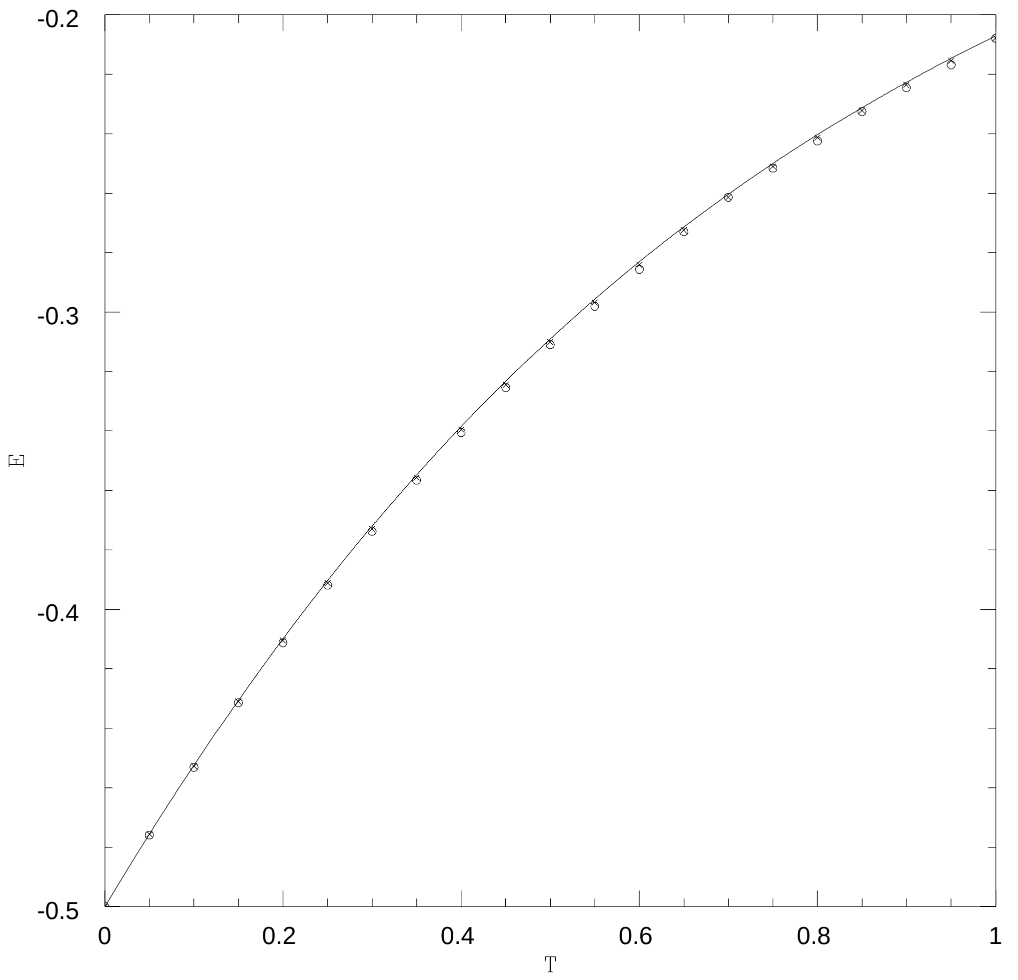

Figure 5: Energy of the fully frustrated hypercubic cell (XY model) for $D = 8$ (empty dots) and $D = 15$ (small $\times$ symbols) as a function of the temperature T. The continuous line is the high temperature prediction. There is no signal of the presence of a phase transition.

Acknowledgments

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